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(54) Title: A METHOD FOR PERFORMING RESTRAINED DYNAMICS DOCKING OF ONE OR MULTIPLE SUBSTRATES ON MULTI-SPECIFIC ENZYMES

(57) Abstract: The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multipspecific and flexible active site. It also concerns a method for determining the 3D-substrates, which is the case for multispecific enzymes such as cytochrome P450, and specifically to cytochrome P450 3A4 and P450 3A7.



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# A method for performing restrained dynamics docking of one or multiple substrates on multi-specific enzymes

The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multispecific and flexible active site. It also concerns a method for determining the 3D-structure of active sites that are flexible and can adapt to different substrates, which is the case for multispecific enzymes such as cytochrome P450.

As of today, various computer graphics systems allow to generate molecular models of large molecules such as proteins from the PDB structural data obtained using X-ray crystallography and NMR. We can cite for example MODELLER, COMPOSER, MATCHMAKER (Tripos), or 3D graphical environments for molecular modeling such as SYBYL (Tripos) or INSIGHT II (Accelrys).

Substrates as well as inhibitors or agonists often act by binding to particular regions of an enzyme or receptor referred as the active site. In industry, the purpose of using these 3D models is to assess the main features of the molecules which are involved in the binding to the active site. New molecules that fit the active site can be designed.

Biological interactions are not possible without flexibility and motion. One of the principal tools in the theoretical study of motion in biological molecules is the method of molecular dynamics simulations (MD). This computational method calculates the time dependent behavior of a molecular system (Karplus and McCammon, 2002). MD simulations have provided detailed information on the fluctuations and conformational changes of proteins and nucleic acids. These methods are now routinely used to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes. They are also used in the determination of structures from x-ray crystallography and from NMR experiments. The molecular dynamics simulations can be used to recreate the successive events in the binding process of a molecule, and thermodynamic parameters implicated in such process can therefore be derived, which is of great interest in the design of active molecules.

Nevertheless, the methods proposed in the art are based on a relatively low level of calculations of few parameters. It relies only on the molecule energy constrained with a fixed geometry. It relies only on the interaction energy between the molecule and the active site frozen in a fixed geometry.

5 Consequently, there is a need for a model replicating *in silico* the natural process of molecular interactions.

The method according to the invention provides both minimizations and molecular dynamics calculations. More specifically, it provides a new approach which is more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained restrained dynamics docking". This technique employs constrained dynamics simulations, where the only constraints are active site-substrate distances.

For example, to explain and predict drug metabolism in organisms, in which the cytochrome P450 (CYP) superfamily of haem-thiolate enzymes plays a central role, it is of large interest to dispose of a molecular picture of the binding sites responsible for the biotransformation. Efficiency of the prediction is then directly related to the molecular precision of the model, which resolution must be obtained at the atomic level to exploit the model for further docking studies.

In mammalian, hepatic cytochrome P450s constitute the major enzymes involved in the metabolism of exogenic compounds. Among them, isozymes of the CYP3 family (such as CYP3A1 and 3A2 in rat, and CYP3A4, CYP3A5, CYP3A7, CYP 3A43 in human) are known to metabolize the majority of drugs in clinical use. These are multi-specific enzymes, able to metabolize a large variety of structurally diverse chemicals or substrates including steroids, linear or cyclized peptides (Delaforge et al. 1997, Delaforge et al. 2001, Aninat et al. 2001), generally fairly lipophilic, within a broad range of molecular sizes from testosterone (Mw 288) to cyclosporin A (Mw 1203).

The inventory of known substrates for CYP 3A contains a large variety of different molecules having apparently no common structural factors. Actually it can be estimated that more than five hundred utilized drugs can be recognized and metabolized by CYP 3A (Guengerich 1995, Wrighton et al. 2000, Lewis 2001). Closer inspection of the precise transformations catalyzed by CYP 3A indicates that there is an important regio- and stereo-selectivity for each substrate. The active site

can accommodate relatively rigid substrates such as aflatoxin derivatives or steroids, that are oxidized almost exclusively at a precise position. Thus CYP 3A4 catalyzes the testosterone oxidation exclusively at the 6β position, whereas CYP 3A7 oxidizes dehydroepiandrosterone (DHEA) or its 3 sulfate conjugate exclusively on the 16α position (see Figures 4A and 4B). In addition to such small substrates, CYP 3A metabolize also large molecules such as cyclosporin A (MW 1202), macrolide antibiotics (MW around 600) or ergot derivatives (MW from 500 to 700).

The recognized substrates can have endogenous origin such as steroids or can be drugs or compounds found in food. For example, grapefruit juice contains bergamottin derivatives having specific CYP 3A inhibitory activities (Schmiedlin-Ren et al. 1997). Linear peptides (Delaforge et al. 2001, Hosea et al. 2000) or cyclized peptides (Delaforge et al. 1997) containing from 2 aminoacids (called diketopiperazine, Delaforge et al. 2001, Aninat et al. 2001) to 11 amino-acids (e.g. cyclosporin) are also recognized.

Following this wide range substrate recognition, a tentative subclassification was established leading to a multi-site hypothesis (Hosea et al. 2000, Ekins et al. 2003) consisting of at least 2 or 3 binding zones in the active site. This hypothesis has been established on the facts that CYP 3A shows often atypical hyperbolic kinetic constants and is thus unable to reach saturation. In addition, the presence in the active site of a second substrate having a different molecular nature lead to either no modification or increased metabolism of both substrates. Such allosteric effects have been clearly described in the case of simultaneous metabolism of steroids such as testosterone and  $\alpha$ -natphtoflavone.

Consequently, any molecular model describing correctly the multiple substrate specificity (that takes into account large variations in molecular size and chemical structures), and substrate cooperativity effects within the active site (when two or more drugs interact), is of considerable scientific and industrial interest. Such a molecular model must be able to rationalize the binding of the diverse known substrates, and the orientations of the molecules in the binding site that account for their known positions of metabolism (such as N-demethylations, benzylic hydroxylations etc.).

CYP3A4 is considered as the main hepatic form and is found in a wide variety of human organs such as intestine, brain or skin. CYP 3A5 is also present in liver and is the major 3A form present in the kidney. The 3A5 isoform is subject to genetic polymorphism. CYP 3A7 is the major 3A isoform present in the foetus whereas CYP3A43 is mainly located in adult prostate or testis. These isoforms share amino acid identities higher than 70%. (Westlind-Johnsson et al. 2003, Gellner et al. 2001, Koch et al. 2002). It is currently accepted that CYP3A4 is the most active isoform for classical P450 3A substrates whereas recent data (Williams et al. 2002) demonstrate equal or slightly reduced activity for CYP3A5 and a significantly lower metabolism capability for CYP3A7 as compared to CYP3A4. Additionally, differences have been observed in term of oxidative regioselectivity of the CYP3A7 compared to other isoforms. As an example, CYP3A7 metabolizes intensively DHEA and especially its sulfate conjugate derivative whereas CYP3A4 is a poor metabolizer. The oxidation by CYP3A7 occurs mostly in the 16a position of DHEA. In contrast, CYP3A7 metabolizes testosterone in both 6β and 16α position whereas CYP3A4 or 3A5 metabolize it almost exclusively in the 6B position (Inoue et al. 2000).

At the contrary of the P450 3A subfamily, other P450 isoforms have more rigid active site, as suggested by the narrow range of recognized substrates or inhibitors.

These P450 isoforms recognize generally a small number of substrates or inhibitors having in common the same shape (i.e. P450 1A isoforms), or the same charge (i.e. CYP 2B, 2C or 2D isoforms), or the same chemical nature such as steroids (i.e. CYP19 or CYP21 isoforms) or lipids (i.e. CYP 4 family).

As no high-resolution 3D structure of CYP3A is today publicly available, due to continuing difficulties in promoting crystallization of intrinsic membrane proteins or due to an unusual conformational flexibility that would explain how CYP3A can accommodate various substrates, it is necessary to rebuild a 3D model structure, integrating the known biochemical data of CYP3A and the structural data of other members of the CYP superfamily. X-ray crystallographic determinations of several bacterial P450 enzymes in the 1990s (see Table 1 for a summary of structural data) have stimulated numerous attempts in modeling microsomal P450S such as human CYP3A4. The chapter 6 of the book "Guide to Cytochromes P450: structure and function" written by David F.V. Lewis reviews the current status of structural and

modeling investigations of the P450 family (Lewis 2001). This review was however written just before the release of the first mammalian P450 structure (2C5), still today the only one mammalian template available.

Table 1

CYP isoform crystallized	PDB code (resol.)	Organism	Function	No of residues	Reference
P450 cam (complexed by CO+camphor)	3cpp (1.9 Å)	Pseudomonas Putida	Camphor Monooxygenase	414	(Poulos et al. 1985) (Raag and Poulos 1989)
P450 terp	1cpt (2.3 Å)	Pseudomonas sp.	Alpha-terpineol hydroxylation	412	(Hasemann et al. 1994)
P450 BM3	2hpd (2 Å)	Bacillus megaterium	Fatty acid monooxygenase	471	(Ravichandran et al. 1993)
P450 cryF (6-deoxyerythro -nolide B bound)	loxa (2.1 Å)	Saccharopolyspora erythraea	Erythromycin biosynthesis 6S- hydroxylation of 6- deoxyerythronolide B	403	(Cupp-Vickery and Poulos 1995)
P450 nor	lrom (2 Å)	Fusarium oxysporum (denitrifying fungus)	Nitric Oxide Reductase	403	(Park et al. 1997)
P450 2C5	1dt6 (3 Å)	(membrane-type Mammalian) Rabbit	Progesterone 21- Hydroxylase	473 (487)	(Williams et al. 2000)
P450 CYP119 4-Phenylimidazole Bound	1f4t (1.93 Å)	Sulfobolus Solfactaricus Thermophilic bact.	unknown	368	(Yano et al. 2000)
P450 CYP51 4-Phenylimidazole Bound	1e9x (2.1 Å)	Mycobacterium Tuberculosis	14 α-sterol demethylase	455 (451)	(Podust et al. 2001)

Table 1: the eight X-ray crystal structures of P450s available in 2002: six bacterial, one fungal (P450 nor), one mammalian (CYP2C5). The P450<sub>cam</sub>, P450<sub>terp</sub>, P450<sub>eryF</sub>, P450<sub>nor</sub> belong to class I P450s enzymes, whereas P450<sub>BM3</sub> belongs to class II enzymes, like microsomal enzymes CYP2C5 and 3A. P450<sub>BM3</sub> structure is therefore a priori more relevant to rebuilding a structural model of CYP3A, but since the CYP2C5 X-Ray structure has been released, it became obvious that the structural homology between the other bacterial enzymes and microsomal enzymes was better than expected from the poor homology of primary structure (< 25% identity). Then, the relevance of using class I and class II structures together for rebuilding models of class II P450s was no more questionable. In the two examples described in the present invention, the structural model of human CYP3A4 was rebuilt using the six

first structures listed above, with no preference in the structural alignment, and the structural model of human CYP3A7 was rebuilt using four structures among those listed above with again no preference in the structural alignment, *i.e.* P450<sub>BM3</sub>, P450 EryF, P450 2C5 and CYP51, one of the last published structural sets. CYP119 was not incorporated into the modeling process.

All the proposed models of CYP3A4 obtained by homology modeling are thus so far based on bacterial crystal structure templates: the first was proposed by Ferenczy and Morris and used the X-ray structure of bacterial P450<sub>cam</sub> as unique template structure (Ferenczy and Morris 1989). Another model was built later by David F.V. Lewis, using also a unique template structure, the P450<sub>BM3</sub> structure, which was supposed to be more relevant as a template since this P450 was the only one class II enzyme with known three-dimensional structure (Lewis et al. 1996). A third model, based on a multiple structure template, was built by Szklarz and Halpert, using the four first X-ray crystal structures available P450cam, P450terp, P450<sub>ervF</sub>, and P450<sub>BM3</sub>. This four-bacterial template approach strategy is closer to our rebuilding strategy, but was still missing some relevance in the absence of a mammalian template. In our hands, the incorporation of the mammalian 2C5 crystal structure into rebuilding steps of models of cytochrome P450 3A proved to be decisive. Inclusion of 2C5 crystal structure had indeed a profound effect on the structural alignment with the five non-mammalian structures, resulting in a different topology of the active site and a marked divergence between the model and each individual template. The advantage of our multiple-template approach resides essentially in the availability of a final template that can be used to rebuild various mammalian cytochromes P450. Up to now there is no available crystal structure or structural model of human CYP3A5, CYP 3A7, CYP3A43 or other mammalian CYP3A.

More recently, two new bacterial P450 crystal structures emerged in the literature (Table 1): CYP51 (PDB code 1e9x), from *Mycobacterium tuberculosis*, that catalyzes the oxidative removal of 14α-methyl group from sterol precursors in sterol biosynthesis in yeast and fungi (ergosterol), plants (phytosterol) and mammals (cholesterol), for its potential in the design of antifungal agents (Podust et al. 2001). And CYP119 (PDB code 1f4t), from the thermophilic archaeon *Sulfolobus solfataricus*, the first P450 identified in *Archaea*, for its interest in

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understanding the enhanced thermal stability of the structure, especially in the region of the active site (Yano et al. 2000). Those two structures have been shown to exhibit the typical bacterial P450 fold, with some exceptions in the topology. They have not been included as structural templates in the modeling steps of the CYP3A4 model described in example 1. The names of newly discovered P450s follow the now accepted nomenclature of David R. Nelson (Nelson 1999).

The protein databank (Brookhaven Protein Databank, http://www.rcsb.org/pdb/) currently indicates that there are 76 separate crystal structures available for the eight crystallized P450s, plus 7 crystal structures on hold (Sept 1st, 2002), the majority of which containing either bound substrates or inhibitors. Table 1 provides the relevant information about the structural templates used for human CYP3A model rebuilding. The idea behind homology modeling is that proteins belonging to the same functional class and showing a strong sequence identity, adopt a similar fold (review in (Hilbert et al. 1993)). Known analogous structures are then used to 15 generate a template or parent structure for the unknown protein to be modeled. The reliability of the various methods employed depend mostly on the number of experimental 3D structures that can be aligned. Knowing that for pairs of distantly related proteins (with residue identity of about 20%) the regions having the same fold will represent less than half of each molecule, the regions where the folds differ will predominate, and the divergence of sequence must be compensated by a higher number of homologous proteins to align (Chothia and Lesk 1986). Below 50% of sequence identity, the deviation in structurally not conserved regions becomes significant, and loop regions are difficult to predict. It is generally accepted that below 20% of sequence identity, the prediction turns out to be hazardous, and fold assignment methods are best replaced by ab initio methods, that ideally attempt to predict the native structure only from the primary sequence of the protein to be modeled. But produced models so far had the correct fold for only a few small protein domains (Sanchez et al. 2000).

The strategy of model rebuilding in the P450 family is strongly driven by the low degree of homology between bacterial and mammal cytochrome P450s (Table 2).

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Fable 2

	ER FUSOX										% 2
	BACME SACER					,				22.6 % [25] 389 aa	23.0 % 32.7 %
-	PSESP BAC								24.0 % 139 363 aa	28.6 % 22. 420 aa 389	
	PSEPU PS							27.4 % 398 aa	23.1 % 24 485 aa 36	25.5 % 26.0 % 27.7 % 30.8 % 24.4 % 24.0 % 28.6 % 415 aa 334 aa 423 aa 396 aa 443 aa 391 aa 420 aa	23.7% 22.9% 23.1% 27.7% 21.4% 29.0% 31.5%
	RABIT P						24.2 % 480 aa	24.4 % 2 451 aa 3		24.4 % 2 443 aa 3	23.7% 22.9% 23.1% 27.7% 21.4% 29.0%
	SULSO   F					23.5 % 344 aa	26.6 % 387 aa	29.3 % 409 aa	24.5 % 22.7 % 396 aa 480 aa	30.8 % 396 aa	27.7 %
CP51_	MYCTU				25.7 % 385 aa	23.4 % 427 aa	23.3 % 21.3 % 21.9 % 26.6 % 335 aa 399 aa 407 aa 387 aa	27.8 % 446 aa	27.1 % 443 aa	27.7 % 423 aa	23.1 %
CP34_	HOMAN	<b>表</b>		27.7 % 26.9 % 372 aa 405 aa	25.4 % 410 aa	28.4 % 497 aa	21.3 % 399 aa	24.4 % 356 aa	29.9 % 445 aa	26.0 % 334 aa	22.9 %
CP37_	HUMAN		88 4 % (50 Caa	27.7 % 372 aa	24.5 % 330 aa	27.9 % 481 aa	23.3 % 335 aa	24.8 % 452 aa	31.8 % 409 aa	25.5 % 415 aa	23.7 %
Swiss-Prot	entry name	CP37_HUMAN	CP34_HUMAN	CP51_MYCTU (CYP51)	CPXW_SULSO (CYP119)	CPC5_RABIT (CYP2C5)	CPXA_PSEPU (P450 cam)	CPXL_PSESP (P450 terp)	CPXB_BACME (P450 BM3)	CPXJ_SACER (P450 eryF)	NOR_FUSOX
P08	epoo	n.s.	n.s.	1E9X	1F4T	1DT6	3CPP	ICPT	2HPD-A	10XA	IROM

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Table 2: Sequence identities between the various crystallized cytochrome P450s and human CYP3A4 and CYP3A7 using BLOSUM 62 matrix (source LALIGN, <a href="http://www.infobiogen.fr/services/analyseq/cgi-bin/lfastap\_in.pl">http://www.infobiogen.fr/services/analyseq/cgi-bin/lfastap\_in.pl</a>, algorithm of Huang and Miller LALIGN that finds the best local alignments between two sequences, version 2.1u03 April 2000, published in *Adv. Appl. Math.* 1991, 12: 373-381). The P450 BM3 structure, Swissprot code name CPXB\_BACME, corresponds to the structure of a fusion protein of P450 and a reductase domain, so that it displays twice the number of residues.

- Our global scheme, which steps are described hereafter, is founded on a combination of methods developed in the literature for different purposes in protein structure determination studies. The principle of the primary steps, until the generation of a correct alignment of P450 primary sequences, is described in Jean et al. 1997. The last steps are summarized in Loiseau 2002.
- Therefore, in a first object, the invention relates to a method for designing a 3-dimentional (3-D) model of a protein, the 3-D representation of at least three family members has already been experimentally obtained, [said 3-D representation presenting similarities], comprising the steps of:
- a. identification of common structural blocks (CSBs) among said members of said family,
  - b. alignment of the amino-acids primary sequence of said family members according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
- c. alignment of said protein as compared on said first alignment, in order to obtain a
   second alignment, wherein:
  - i. alignment of said protein is performed in order to optimize the amino-acids alignment between said protein and said first alignment, when one or more consensus amino-acid exists in said aligned CSBs in said first alignment, and in the amino-acid sequence of said protein, said consensus amino-acids are anchors of said second alignment,
  - ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible in out-of-block regions, if better to align the primary amino-acids sequences,

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- d. definition of the 3-D structure of CSBs of said protein, according to the 3-D structure of the CSBs of said family members,
- c. definition of the global constraints (distance and angular constraints) derived from the comparisons of the structural templates in CSBs, and definition of the local constraints (distance and angular constraints) for the atoms of residues that are not structurally determined after step d. (that are not in the CSBs),
- f. selection of rotamers,

mutations having biological effects.

- g. determination of a family of 3-D model structures of said protein, taking into account said 3-D structure of CSBs obtained in step d., said global and local constraints defined in step e., and said rotamers defined in step f.,
- h. optimization of said family of 3-D models obtained in step g., by
- i discarding structures that present topological defects, and
- ii recalculating 3-D structures by taking electrostatic forces into account, and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment, when the obtained model structures do not satisfactorily account for known
- In the present invention, the term "backbone atoms" refers to the C, N, C $\alpha$ , and O atoms of a protein that are common to all amino acid building blocks or involved in the peptide linkage. When the protein structure is described as a trajectory in internal coordinates such as  $\alpha$ ,  $\tau$  angles, or is a low-resolution crystallographic structure, backbone atoms stand only for C $\alpha$  atoms of each residue.
- In the present invention, the term "similarities" is used in the search for structural fragments conserved between the template proteins, that is fragments that have similar local trajectories in the backbone internal coordinate space. Two protein fragments have "similar" local trajectories when they are matched according to two adjustable parameters, the mesh and the margin (Jean et al. 1997).
- In the present invention, the term "common structural blocks (CSB)" define the protein fragments of equal length that are found similar between all the template proteins in the internal coordinate representation.
- In the present invention, the term "first alignment" refers to the alignment imposed by the CSBs, that is the structural alignment between template proteins defined by

CSBs sequences. This alignment is totally independent on the primary sequence of the template proteins.

In the present invention, the term "out-of-block regions" designates all other protein fragments located out of and between the CSBs, *i.e.* that are not structurally conserved in the internal coordinate space. There is no information of sequence alignment for these regions (see in Figure 1 regions that are not colored), since they are not relevant for structural conservation. Out-of-block regions are passively reconstructed with the rest of the structure during the calculation steps.

In the present invention, the term "global constraints" refers to geometric constraints that are assigned to atoms of residues from CSBs, and that can be derived by computing all distance or angle information available within CSBs or between CSB.

In the present invention, the term "local constraints" refers to loose structural constraints that are assigned to residues of out-of-block regions, in order to restrict their backbone conformation to allowed regions of the Ramachandran diagram.

In the present invention, the term "rotamers" defines the low energy side-chain conformations of residues. The use of a library of rotamers allows determining or modeling a structure with the most likely side-chain conformations, saving time and producing a structure that is more likely to be correct.

20 For identification of CSBs between all selected 3D structures:

CSBs define the common local folds found similar in the template proteins, and are used as building blocks to set up the fold of the model (results in Loiseau 2002). The non conserved regions, that can be parts of secondary structures or non-structured regions as loops, will be rebuilt with no initial structural information.

For multiple alignment of crystalline P450s, on the basis of CSBs determination:

Once the structurally conserved elements are identified, a first structural alignment between the template proteins is derived. The following step involves the localization of these elements in the target sequence. Sequence pairwise comparisons between selected crystal structures and CYP3A (Table 2) show low sequence identity, so that online tools of multiple alignment such as CLUSTALW or PHD (Heidelberg) fail to produce an clear-cut alignment. Instead, local alignment tools, such as that described in Jean et al. 1997, were used to match the CSB profile to the target sequence, where a matrix is slid along the sequence and a

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score of similarity (based on a standard matrix such as BLOSUM62) is calculated for each position. Online tools of multiple alignment such as CLUSTALW 1.8 can be further used for assessment of accuracy.

The target sequence of human cytochrome P450 3A is thus aligned against the multiple alignment obtained from the CSBs. This produces the key sequence alignment which allows the generation of the template structure used for the rebuilding of the various CYP3A models. Following steps involve:

- 1) Generation of distance and dihedral angles constraints.
- 2) Selection of rotamers for side chains in CSBs.
- 3) Calculation of a set of structures using DYANA software. Loops are rebuilt between CSBs.
  - 4) Structure optimization under XPLOR software (Brünger 1992).

In a preferred embodiment, said 3-D representation of family members has been obtained by crystallography or NMR.

The alignment of said common structural blocks in steps **b**. and **c**. can be performed by use of the GOK software as described in Jean et al., 1997.

In addition, step d. is preferably performed according to the following rules:

- i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the target residue,
- ii. When residues differ, only the coordinates of the backbone atoms are assigned  $(C\alpha)$ , and sometimes  $C\beta$  or  $C\gamma$  when they exist.

The definition of rebuilding global constraints in step e. is performed by using all available geometrical information intra- and inter-CSB (distances and angles), issued from the comparisons of the structural templates, each geometric constraint being defined as an interval. On another hand, the definition of local constraints for out-of-blocks residues is performed by analysis of the allowed regions in Ramachandran diagram.

Furthermore, distances and angles defining global constraints are preferably selected in step e. by the following rules:

- i. all distances for which the lower boundary is less than 8 Å,
- ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs

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iii.all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom

The distance of 8 Å is chosen in order to reduce drastically the total number of constraints to take into account in the computation, and to allow to excessively constrain the model.

Angular constraints are preferably selected in step e. by the following rule:

i. dihedral angles  $\phi$  and  $\psi$  of all residues located in CSBs are defined as constraints, given by the average values of corresponding  $\phi$ ,  $\psi$  angles in said family members +/- the calculated standard deviation.

To practice the method of the invention, rotamers in step f. can be selected from the couples according to the tables of Dunbrack and Karplus and step g. can be performed with the DYANA software, as described in Güntert et al, 1997.

In addition, the optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brünger, X-PLOR, version 3.1.

The method according to the invention is particularly applicable to a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A]

In a preferred embodiment, said mammal cytochrome P450 3A is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18)

0 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).

In another preferred embodiment, said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).

The method is applicable as well to human cytochrome of the subfamily P450 3A4, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A4 are chosen from Nor (SEQ ID N° 1), Ery F (SEQ ID N° 2), terp (SEQ ID N° 3), Cam (SEQ ID N° 4), BM3 (SEQ ID N° 5) and 2C5 (SEQ ID N° 6).

The method is applicable as well to human cytochrome of the subfamily 3A7, wherein family members that are used for performing said first alignment for designing a 3-D model of CYP3A7 are chosen from Ery F (SEQ ID N° 2), BM3 (SEQ ID N° 5), CYP51 (SEQ ID N° 8) and 2C5 (SEQ ID N° 6).

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The method is applicable as well to other mammalian cytochrome P450 3A isoforms.

In a second object, the invention is directed to 3-D structure model of a protein, obtained by the method as described above.

- In a preferred embodiment, the protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A

  In another preferred embodiment, the protein is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
- In still another preferred embodiment, the protein is a human cytochrome P450 subfamily 3A selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13). In still another preferred embodiment, the protein is a human cytochrome P450 3A4 or 3A7.
- Regarding the rebuilt P450 3A4 model, the main residues involved in the recognition of the substrate are C97; R104; F101; F107; F247; F303 and C376. More specifically, C97 and C376 are found in positions compatible with the formation of a disufide bridge allowing limited or enhanced flexibility of corresponding protein domains, while R104 is involved in the capture of the substrate that is close to the entrance site, and allows to accompany it to the active site. F303 is involved in the recognition of the substrate in the active site. F107; F247 and F303 are involved in the recognition at the modulation site responsible for positive regulation. Role of F303 in the active site has already been suggested by studies of Domanski et al. 1998 in the SRS 4 region (mutants I300, F303, A304, and T308).

Features of this model comprise the 3-D atomic coordinates of Table 3.

Table 3

In a preferred embodiment, the residues C97; R104; F101; F107; F247; F303 and C376 are involved in the CYP 3A4 for the recognition and uptake of the substrate at the entry site, and its binding into the active site having the 3-D atomic coordinates of Table 3.

Regarding the P450 3A7 model, features comprise the 3-D atomic coordinates of **Table 4**.

### Table 4

In a preferred embodiment the residues Q79; F102; R105; R106; F108; F248; F304 and E374 are involved in the CYP 3A7 for the recognition and uptake of the substrate at the entry site, and its binding into the active having the 3-D atomic coordinates of Table 4.

In a third object, the invention contemplates a method for designing a protein, biological functions of which are altered, comprising:

- a) obtaining a 3-D model of said protein by the method as depicted above,
- b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
  - c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.

In the present invention, the term "altered properties" means that the generated protein is altered in its enzymatic properties, such as the substrate recognition, the movements associated to the entrance or the exit of the substrate, the multiple binding at the active site, the allosteric behaviour, the electron transfer, the coupling to the P450 reductase.

In another object, the invention relates to a computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps:

- j. determining a force field, and independently simulating the presence of said enzyme in said force field,
- k. minimizing the potential energy (Ep) linked to said force field of said 3-D structure, wherein the spatial position of some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by i. simulating an increase in temperature (in order to give kinetic energy), ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- 30 I. optionally repeating step k in order to obtain other Ep minima, wherein said Ep minima are such that the structure of the protein remains folded,
  - m. minimizing Ep in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by

- i. simulating an increase in temperature (in order to give kinetic energy), and
- ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- simulating, at 0 K the presence of said substrate next to said enzyme,
- optionally generating a molecular dynamics simulation on said substrate and 0. enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)
- generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- generating a molecular dynamics simulation on said substrate and enzyme, with said constraints imposed in step p., 10
  - optionally, generating a molecular dynamics simulation on said substrate and enzyme without said constraints of step p.
  - In the present invention, the term "restrained dynamics docking" means a procedure by which the docking of the substrate is simulated using molecular dynamics (MD) simulations under constraints that are specified by the user.
  - In the present invention, the term "soft-restrained dynamics docking" refers to a restrained dynamics docking in which the substrate-protein distance constraints are loose, with force field parameters associated to the constraints as low as 1 or 2 Kcal/mol.
- In the present invention, the term "constraints" when applied to substrate docking refers to a distance imposed between atoms of the protein, generally from the active site (such as atoms of the heme group), and atoms of the substrate. These distance restraints are defined as intervals, where the distance range is large enough to allow the free movement of the substrate within the active site.
- In a preferred embodiment of this method for performing restrained dynamics docking, said fixed atoms in step k. are the backbone atoms N-Ca-CO in the first minimization step and only  $C\alpha$  in subsequent minimization steps.
  - In another preferred embodiment of this method, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
- The force field in step j. comprises forces linked to: 30
  - a. the distance between atoms,
  - b. the angles of valence,
  - c. the dihedral angles,

- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- g. hydrogen bonds.
- The constraints in step **p**. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- In the present invention, the term "final distance constraints", when applied to substrate docking, means distances imposed between atoms from the heme group (such as the iron atom), and atoms of the substrate. These distance contraints are defined as intervals, and are related to the final position of the substrate in the vicinity of the heme group before metabolization.
- 15 Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.
  - This method is particularly suited for multispecific protein such as a cytochrome 36 P450 subfamily 3A comprising mammal and human cytochromes.
    - The cytochrome can be cytochrome P450 3A4 or any of all other P450 from the 3A subfamily, and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.
- The substrate can be a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).
  - In a preferred embodiment said substrate is testosterone.
  - In another object, the invention is aimed at a computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a
  - 3-D structure of which is available, consisting of performing the steps **j**, **k**, **l**, **m**, **n**, **o**, **p**, **q** and **r** depicted above with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained state after molecular dynamics simulations.

The first and second substrates can be the same molecule or different molecules.

The first and second substrates can display either allosteric or synergistic effect.

This method can be practiced with substrates that are inhibitors (competitive, uncompetitive, non competitive) or display an inhibitor-base mechanism. It can also

5 be practiced with an agonist and any molecule interfering with the biological function of the protein.

In preferred embodiments:

- the first and second substrates are the same molecule.
- the first and second substrates are different molecules.
- 10 the first and second substrates display an allosteric effect.
  - the first and second substrates display a synergistic effect.
  - at least one of the substrates is an inhibitor or display an inhibitor-based mechanism.
  - at least one of the substrates is an agonist.
- In another embodiment, this method also embraces a successive repeat of the steps j, k, l, m, n, o, p, q and r depicted above with a 3<sup>rd</sup>, 4<sup>th</sup> or 5<sup>th</sup> substrate, some of them being the same or different molecules.

In this method for performing restrained dynamics docking, said fixed atoms in step  $\mathbf{k}$ . are the backbone atoms N-C $\alpha$ -CO in the first minimization step and only C $\alpha$  in subsequent minimization steps.

In addition, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

The force field in step i. comprises preferably forces linked to

- a. the distance between atoms,
- 25 b. the angles of valence,

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- c. the dihedral angles,
- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- 30 g. hydrogen bonds.

The constraints in step p. are preferable attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance

constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.

Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome P450. The cytochrome can be cytochrome P450 3A4, or any of all other P450 of the 3A subfamily and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.

In a preferred embodiment:

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- said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the above-described method, in particular the above-described model structure,
- said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A),
- said substrate is testosterone.

The invention is also directed to the use of the method for designing a 3-D model of a protein and to the computer-assisted method for performing restrained dynamics docking as mentioned above for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.

Another object of the invention is the use of these methods for determining the effect of a first substrate on a second substrate, which can also be applied to pharmaceutical products.

The invention contemplates the use of these methods for determining the effect of a first bound testosterone molecule on the access of a second testosterone molecule as well as for determining the mutual effect of a testosterone molecule with alphanaphtoflavone ( $\alpha$ NF) molecule.

The invention is also directed to:

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- \* The use of the above described computer-assisted methods for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate to give rise to metabolite.
- The oxidized or reduced molecule derived from a given substrate modified after positioning at the right distance to the heme is called metabolite.
  - \* The use of the above described computer-assisted methods, for performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the calculation.
- \* The use of the above described computer-assisted methods for dynamic docking to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to determine if the exit of the given metabolite from the enzyme is favored or not.
  - \* The use of the above described computer-assisted methods for dynamic docking to study the different exit pathways that are accessible to the metabolite, either in the absence or in the presence of the second substrate in the calculation.

15

The distance and angular constraints derived from CSBs common to the crystallized cytochromes P450 used as structural templates, are applied to conserved atoms of CSBs of the target protein. The DYANA software (Güntert et al. 1997) allows to rebuild directly the whole structure of the target protein on the basis of its primary sequence, by taking into account these geometric constraints. Out-of-blocks residues are rebuilt *ab initio* by selecting the most favorable solutions in terms of minimal global potential energy. As examples, actual tables 3 and 4 display the atomic coordinates of structural models obtained by applying DYANA calculation to target protein sequences CYP3A4 and CYP3A7 respectively.

```
TABLE 3 :Providing the coordinates of the CYP3A4 model
          CYP3A4
HEADER
          MODEL OF HUMAN CYTOCHROME P450 CYP3A4
TITLE
             LOISEAU, F. ANDRE, C. MINOLETTI, M. DELAFORGE
AUTHOR
                   SER TYR HIS LYS GLY PHE CYS MET PHE ASP MET GLU CYS
SEQRES
                    HIS LYS LYS TYR GLY LYS VAL TRP GLY PHE TYR ASP GLY
SEORES
                    GLN GLN PRO VAL LEU ALA ILE THR ASP PRO ASP MET ILE
SEQRES
              452
         3
                    LYS THR VAL LEU VAL LYS GLU CYS TYR SER VAL PHE THR
              452
SEQRES
         4
                    ASN ARG ARG PRO PHE GLY PRO VAL GLY PHE MET LYS SER
              452
SEQRES
         5
                    ALA ILE SER ILE ALA GLU ASP GLU GLU TRP LYS ARG LEU
         6
               452
SEQRES
                    ARG SER LEU LEU SER PRO THR PHE THR SER GLY LYS LEU
         7
               452
SEQRES
                    LYS GLU MET VAL PRO ILE ILE ALA GLN TYR GLY ASP VAL
SEQRES
         8
               452
                    LEU VAL ARG ASN LEU ARG ARG GLU ALA GLU THR GLY LYS
SEQRES
               452
                    PRO VAL THR LEU LYS ASP VAL PHE GLY ALA TYR SER MET
               452
SEORES
        10
                    ASP VAL ILE THR SER THR SER PHE GLY VAL ASN ILE ASP
               452
SEORES
        11
                    SER LEU ASN ASN PRO GLN ASP PRO PHE VAL GLU ASN THR
SEQRES
        12
               452
                    LYS LYS LEU LEU ARG PHE ASP PHE LEU ASP PRO PHE PHE
SEQRES
        13
               452
                    LEU SER ILE THR VAL PHE PRO PHE LEU ILE PRO ILE LEU
SEQRES
        14
               452
                    GLU VAL LEU ASN ILE CYS VAL PHE PRO ARG GLU VAL THR
        15
               452
SEQRES
                    ASN PHE LEU ARG LYS SER VAL LYS ARG MET LYS GLU SER
               452
SEQRES
        16
                    ARG LEU GLU ASP THR GLN LYS HIS ARG VAL ASP PHE LEU
SEQRES
        17
               452
                    GLN LEU MET ILE ASP SER GLN ASN SER LYS GLU THR GLU
SEORES
        18
               452
                    SER HIS LYS ALA LEU SER ASP LEU GLU LEU VAL ALA GLN
SEQRES
        19
               452
                    SER ILE ILE PHE ILE PHE ALA GLY TYR GLU THR THR SER
        20
               452
SEORES
                    SER VAL LEU SER PHE ILE MET TYR GLU LEU ALA THR HIS
               452
SEORES
        21
                    PRO ASP VAL GLN GLN LYS LEU GLN GLU GLU ILE ASP ALA
SEQRES
        22
               452
                    VAL LEU PRO ASN LYS ALA PRO PRO THR TYR ASP THR VAL
SEQRES
         23
               452
                    LEU GLN MET GLU TYR LEU ASP MET VAL VAL ASN GLU THR
         24
               452
SEORES
                    LEU ARG LEU PHE PRO ILE ALA MET ARG LEU GLU ARG VAL
               452
SEQRES
         25
                    CYS LYS LYS ASP VAL GLU ILE ASN GLY MET PHE ILE PRO
SEQRES
         26
               452
                    LYS GLY TRP VAL VAL MET ILE PRO SER TYR ALA LEU HIS
               452
SEORES
         27
                    ARG ASP PRO LYS TYR TRP THR GLU PRO GLU LYS PHE LEU
SEQRES
         28
               452
                    PRO GLU ARG PHE SER LYS LYS ASN LYS ASP ASN ILE ASP
SEORES
               452
         29
                    PRO TYR ILE TYR THR PRO PHE GLY SER GLY PRO ARG ASN
         30
               452
SEQRES
                    CYS ILE GLY MET ARG PHE ALA LEU MET ASN MET LYS LEU
SEORES
         31
               452
                    ALA LEU ILE ARG VAL LEU GLN ASN PHE SER PHE LYS PRO
SEQRES
         32
               452
                    CYS LYS GLU THR GLN ILE PRO LEU LYS LEU SER LEU GLY
SEQRES
         33
               452
                    GLY LEU LEU GLN PRO GLU LYS PRO VAL VAL LEU LYS VAL
SEORES
               452
                    GLU SER ARG ASP GLY THR VAL SER GLY ALA
SEQRES
         35
               452
               600
HET
HETNAM HEM
               HEME
               3,7,12,17-TETRAMETHYL-8,13-DIVINYL-2,18-PORPHINEDIPROPIONIC ACID
HETSYN HEM
               C34 H34 N4 O4 FE1
FORMUL HEM
                                   9.999 -1.760 -4.543 1.00
                                                                  0.00
                          51
                  SER
              N
ATOM
                                                           1.00
                                                                  0.00
                                                                                3A4
                                                  -4.293
                                  10.718
                                           -0.477
                          51
ATOM
           2
              CA
                  SER
                                                                                3A4
                                                           1.00
                                                                  0.00
                                   9.949
                                            0.731
                                                   -4.939
                          51
MOTA
           3
              CB
                  SER
                                                                                3A4
                                                                  0.00
                                   8.601
                                            0.876
                                                   -4.493
                                                           1.00
ATOM
           4
              OG
                  SER
                          51
                                                                                3A4
                                                                  0.00
                                  10.962
                                           -0.281
                                                   -2.815
                                                            1.00
           5
              С
                   SER
                          51
ATOM
                                                                                3A4
                                                   -1.969
                                                            1.00
                                                                  0.00
                                           -0.855
                                  10.277
MOTA
              0
                   SER
                          51
                                                                                3A4
                                                            1.00
                                                                  0.00
                                  11.974
                                           0.569
                                                   -2.482
              N
                   TYR
                          52
 MOTA
                                                                                3A4
                                            0.860
                                                                  0.00
                                                   -1.131
                                                            1.00
                          52
                                  12.433
           8
              CA
                  TYR
 MOTA
                                                                                3A4
                                                                  0.00
                                            0.783
                                                   -0.979
                                                            1.00
                                  13.983
              СВ
                   TYR
                          52
           9
 MOTA
                                                                                3A4
                                                            1.00
                                                                  0.00
                                           -0.572
                                                   -1.430
                                  14.459
                          52
              CG
                   TYR
 MOTA
          10
                                                                                3A4
                                                            1.00
                                                                  0.00
                                  14.143
                                           -1.732
                                                   -0.699
                          52
              CD1
                  TYR
 ATOM
          11
                                                            1.00
                                                                  0.00
                                                                                3A4
                                  15.210
                                           -0.701
                                                   -2.611
                          52
              CD2 TYR
 ATOM
          12
                                                                  0.00
                                                                                3A4
                                                            1.00
                                  14.574
                                           -2.994
                                                   -1.138
                          52
 ATOM
          13
              CE1 TYR
                                                                  0.00
                                                                                3A4
                                           -1.954
                                                    -3.052
                                                            1.00
                                  15.651
                          52
 ATOM
          14
              CE2 TYR
                                                                                3A4
                                                                  0.00
                                   15.334
                                           -3.105
                                                    -2.314
                                                            1.00
              CZ
                   TYR
                          52
 ATOM
          15
                                                                                3A4
                                                                  0.00
                                   15.784
                                           -4.370
                                                    -2.751
                                                            1.00
                   TYR
                          52
 MOTA
          16
              OH
                                                                                3A4
                                   11.971
                                                    -0.755
                                                            1.00
                                                                  0.00
                                            2.246
                          52
 MOTA
          17
              С
                   TYR
                                                                   0.00
                                                                                3A4
                                                    -1.494
                                                            1.00
                                            3.208
                                   12.178
          18
              0
                   TYR
                          52
 MOTA
                                                                                3A4
                                                            1.00
                                                                   0.00
                                            2.350
                                                     0.429
                   HIS
                          53
                                   11.321
 ATOM
              N
          19
                                                            1.00
                                                                   0.00
                                                                                3A4
                                                     0.953
                                   10.747
                                            3.568
                   HIS
                          53
              CA
 ATOM
          20
                                                                                 3A4
                                                            1.00
                                                                   0.00
                                                     1.039
                          53
                                    7.857
                                            1.850
              ND1 HIS
 MOTA
          21
                                                                                 3A4
                                                     0.097
                                                            1.00
                                                                   0.00
                                    8.485
                                            2.636
                          53
 ATOM
          22
              CG
                   HIS
                                                                                 3A4
                                                     0.386
                                                            1.00
                                                                   0.00
                                            3.861
                          53
                                    9.322
 ATOM
          23
              CB
                   HIS
                                                                   0.00
                                                                                 3A4
                                                            1.00
                                            0.923
                                                    -0.936
                                    7.438
                          53
 MOTA
              NE2 HIS
          24
                                                                                 3A4
                                                                   0.00
                                            2.053
                                                    -1.104
                                                            1.00
                                    8.216
          25
               CD2 HIS
                          53
 ATOM
                                                                   0.00
                                                                                 3A4
                                                     0.368
                                                            1.00
                                    7.247
                                            0.842
              CE1 HIS
                           53
 ATOM
          26
                                                                   0.00
                                                                                 3A4
                                   10.751
                                             3.386
                                                     2.448
                                                            1.00
                   HIS
                           53
          27
              C
 MOTA
                                                     3.080
                                                             1.00
                                                                   0.00
                                                                                 3A4
                                    9.715
                                             3.183
                           53
          28
              0
                   HIS
 ATOM
                                                                   0.00
                                                                                 344
                                                            1.00
                                                     3.043
              N
                   LYS
                           54
                                   11.973
                                             3.461
           29
 ATOM
```

ATOM	30	CA	LYS	54	12.265	3.262	4.451	1.00	0.00	3A4
ATOM	31	СВ	LYS	54	13.401	2.217	4.659	1.00	0.00	3A4
MOTA	32	CG	LYS	54	13.053	0.819	4.120	1.00	0.00	3A4 3A4
MOTA	33	CD	LYS	54	14.220 14.793	-0.183 -0.500	4.148 5.540	1.00	0.00	3A4
MOTA	34 35	CE NZ	LYS LYS	5 <i>4</i> 54	13.763	-1.087	6.431	1.00	0.00	3A4
ATOM ATOM	36	C	LYS	54	12.660	4.603	5.025	1.00	0.00	3A4
ATOM	37	ŏ	LYS	54	13.829	4.851	5.317	1.00	0.00	3A4
ATOM	38	N	GLY	55	11.656	5.510	5.181	1.00	0.00	3A4
ATOM	39	CA	GLY	55	11.819	6.901	5.560	1.00	0.00	3A4
MOTA	40	С	GLY	55	11.464	7.113	7.003	1.00	0.00	3A4 3A4
ATOM	41	0	GLY PHE	55 56	10.305 12.502	7.002 7.439	7.400 7.817	1.00	0.00	 3A4
ATOM ATOM	42 43	N CA	PHE	56	12.451	7.714	9.250	1.00	0.00	3A4
ATOM	44	CB	PHE	56	13.646	7.051	10.010	1.00	0.00	3A4
ATOM	45	CG	PHE	56	13.966	5.681	9.448	1.00	0.00	3A4
ATOM	46		PHE	56	15.250	5.415	8.926	1.00	0.00	3A4
ATOM	47		PHE	56	12.987	4.669	9.370	1.00	0.00	3A4 3A4
ATOM	48		PHE	56	15.543	4.185 3.445	8.320 8.747	1.00	0.00	3A4
ATOM ATOM	49 50	CE2	PHE	56 56	13.271 14.550	3.205	8.224	1.00	0.00	3A4
ATOM	51	c	PHE	56	12.446	9.211	9.542	1.00	0.00	3A4
ATOM	52	ŏ	PHE	56	11.957	9.670	10.570	1.00	0.00	3A4
ATOM	53	N	CYS	57	12.971	10.054	8.624	1.00	0.00	3A4
ATOM	54	CA	CYS	57	13.048	11.500	8.782	1.00	0.00	3A4
ATOM	55	СВ	CYS	57	13.902 15.312	12.161	7.665 7.176	1.00	0.00	3A4 3A4
ATOM	56 57	SG C	CYS	57 57	11.705	11.121 12.171	8.760	1.00	0.00	3A4
ATOM ATOM	58	Ö	CYS	5 <i>7</i>	11.446	13.160	9.434	1.00	0.00	3A4
ATOM	59	N	MET	58	10.778	11.585	7.975	1.00	0.00	3A4
ATOM	60	CA	MET	58	9.402	12.000	7.870	1.00	0.00	3A4
MOTA	61	CB	MET	58	8.715	11.289	6.694	1.00	0.00	3A4
ATOM	62	CG	MET	58	9.360	11.641	5.343 3.887	1.00	0.00 0.00	3A4 3A4
ATOM	63 64 -	SD CE	MET MET	58 58	8.469 8.922	11.004 9.256	4.080	1.00	0.00	3A4
ATOM ATOM	65	C	MET	58	8.612	11.706	9.122	1.00	0.00	3A4
ATOM	66	ŏ	MET	58	7.740	12.480	9.487	1.00	0.00	3A4
ATOM	67	N	PHE	59	8.963	10.612	9.844	1.00	0.00	3A4
ATOM	68	CA	PHE	59	8.394	10.230	11.122	1.00	0.00	3A4 3A4
ATOM	69	CB	PHE	59	8.732 7.865	8.752 8.152	11.449 12.538	1.00	0.00	3A4
ATOM ATOM	70 71 -	CG	PHE	59 59	6.477	8.002	12.350	1.00	0.00	3A4
ATOM	72		PHE	59	8.430	7.747	13.764	1.00	0.00	3A4
ATOM	73		PHE	59	5.671	7.462	13.364	1.00	0.00	3A4
MOTA	74	CE2	PHE	59	7.627	7.208	14.780	1.00	0.00	3A4
MOTA	75	CZ	PHE	59	6.247	7.065	14.579	1.00	0.00	3A4 3A4
ATOM	76	C	PHE	59 50	8.881 8.110	11.119 11.479	12.255 13.139	1.00	0.00	3A4
ATOM ATOM	77 78	O N	PHE	59 60	10.162	11.568		1.00	0.00	3A4
ATOM	79	CA	ASP	60	10.690	12.515	13.200	1.00	0.00	3A4
ATOM	80	CB	ASP	60	12.225	12.651	13.131	1.00	0.00	3A4
MOTA	81	CG	ASP	60	12.906	11.313	13.450	1.00	0.00	3A4
ATOM	82	_	ASP	60	12.613	10.736	14.532 12.624	1.00	0.00 0.00	3A4 3A4
ATOM	83 84		ASP ASP	60 60	13.743	10.859 13.900	13.031	1.00	0.00	3A4
ATOM ATOM	85	С О	ASP	60	9.841	14.603	14.000	1.00	0.00	3A4
ATOM	86	N	MET	61	9.809	14.318	11.780	1.00	0.00	3A4
ATOM	87	CA	MET	61	9.130	15.564	11.481	1.00	0.00	3A4
MOTA	88	СВ	MET	61	9.224	15.881	9.987	1.00	0.00	3A4
MOTA	89	CG	MET	61	10.590	16.349 16.502	9.497 7.686	1.00	0.00	3A4 3A4
ATOM	90 91	SD	MET	61 61	10.659 12.223	17.411	7.689	1.00	0.00	3A4
ATOM ATOM	92	C	MET	61	7.653	15.548	11.870	1.00	0.00	3A4
ATOM	93	ŏ	MET	61	7.073	16.551	12.274	1.00	0.00	3A4
ATOM	94	N	GLU	62	7.012	14.358	11.819	1.00	0.00	3A4
MOTA	95	CA	GLU	62	5.653	14.159		1.00	0.00	3A4 3A4
ATOM	96	CB	GLU	62 62	5.077 4.640	12.770 12.657	11.933 10.462	1.00	0.00	3A4
ATOM	97 98	CG CD	GLU GLU	62 62	4.351	11.190	10.462	1.00	0.00	3A4
MOTA MOTA	99		GLU	62	3.429	10.603	10.748	1.00	0.00	3A4
ATOM	100		GLU	62	5.048	10.637	9.227	1.00	0.00	3A4
ATOM	101	C	GLU	62	5.522	14.338	13.751	1.00	0.00	3A4

ATOM	102	0	GLU	62	4.508	14.819	14.225	1.00	0.00	3A4
ATOM	103	N	CYS	63	6.605	14.104	14.522	1.00	0.00	3A4
ATOM	104	CA	CYS	63	6.664	14.441	15.921	1.00	0.00	3A4
ATOM	105	СВ	CYS	63	7.902	13.805	16.588	1.00	0.00	3A4
ATOM	106	SG	CYS	63	7.977	11.995	16.382	1.00	0.00	3A4
ATOM	107	С	CYS	63	6.526	15.952	16.211	1.00	0.00	3A4
ATOM	108	0	CYS	63	6.277	16.322	17.335	1.00	0.00	3A4
ATOM	109	N	HIS	64	6.436	16.853	15.182	1.00	0.00	3A4
ATOM	110	CA	HIS	64	5.487	17.970	15.236	1.00	0.00	3A4
ATOM	111	ND1		64	4.140	20.440	16.744	1.00	0.00	3A4
ATOM	112	CG	HIS	64	5.232	20.460	15.904	1.00	0.00	3A4
ATOM	113	CB	HIS	64	6.151	19.284	15.666	1.00	0.00	3A4
ATOM	114	NE2	HIS	64	4.280	22.506	15.939	1.00	0.00	3A4
ATOM	115	CD2		64	5.301	21.731	15.420	1.00	0.00	3A4
ATOM	116	CEL	HIS	64	3.608	21.687	16.726	1.00	0.00	3A4
ATOM	117	С	HIS	64	4.780	18.138	13.901	1.00	0.00	3A4
ATOM	118	0	HIS	64	3.812	17.438	13.610	1.00	0.00	3A4
ATOM	119	N '	LYS	65	5.240	19.107	13.073	1.00	0.00	3A4
ATOM	120	CA	LYS	65	4.699	19.426	11.766	1.00	0.00	3A4
ATOM	121	СВ	LYS	65	3.264	20.052	11.761	1.00	0.00	3A4
ATOM	122	CG	LYS	65	2.994	21.171	12.783	1.00	0.00	3A4
ATOM	123	CD	LYS	65	1.557	21.704	12.722	1.00	0.00	3A4
ATOM	124	CE	LYS	65	1.220	22.723	13.820	1.00	0.00	3A4
ATOM	125	NZ	LYS	65	2.052	23.944	13.700	1.00	0.00	3A4
ATOM	126	C	LYS	65	5.705	20.365	11.146	1.00	0.00	3 <b>A</b> 4
ATOM	127	ŏ	LYS	65	5.958	20.315	9.944	1.00	0.00	3A4
ATOM	128	N	LYS	66	6.332	21.227	12.000	1.00	0.00	3A4
ATOM	129	CA	LYS	66	7.517	22.020	11.730	1.00	0.00	3A4
ATOM	130	СВ	LYS	66	7.373	23.548	12.037	1.00	0.00	3A4
ATOM	131	ÇĞ	LYS	66	6.519	24.352	11.039	1.00	0.00	3A4
ATOM	132	CD	LYS	66	5.001	24.175	11.175	1.00	0.00	3A4
ATOM	133	CE	LYS	66	4.191	25.119	10.278	1.00	0.00	3A4
ATOM	134	NZ	LYS	66	2.736	24.881	10.442	1.00	0.00	3A4
ATOM	135	C	LYS	66	8.551	21.370	12.620	1.00	0.00	3A4
ATOM	136	0	LYS	66	9.100	20.332	12.253	1.00	0.00	3A4
ATOM	137	N	TYR	67	8.772	21.934	13.838	. 1.00	0.00	3A4
ATOM	138	CA	TYR	67	9.441	21.263	14.936	1.00	0.00	3A4
ATOM	139	СВ	TYR	67	11.005	21.348	14.926	1.00	0.00	3A4
ATOM '	140	CG	TYR	67	11.555	20.265	14.028	1.00	0.00	3A4
ATOM	141	CD1	TYR	67	11.325	18.909	14.336	1.00	0.00	3A4
ATOM	142	CD2	TYR	67	12.250	20.569	12.847	1.00	0.00	3A4
ATOM	143	CE1	TYR	67	11.798	17.884	13.506	1.00	0.00	3A4
ATOM	144	CE2	TYR	67	12.720	19.550	12.006	1.00		3A4
ATOM	145	CZ-	TYR	67	12.507	18.207	12.342	1.00	0.00	3A4
ATOM	146	OH	TYR	67	13.010	17.184	11.509	1.00	0.00	3A4
ATOM	147	C	TYR	67	8.880	21.880	16.194	1.00	0.00	3A4
ATOM	148	0	TYR	67	8.905	23.092	16.404	1.00	0.00	3A4
MOTA	149	N	GLY	6 <b>8</b> -	8.343	20.969	17.043	1.00	0.00	3A4
ATOM	150	CA	GLY	68		21.161	18.278	1.00	0.00	. 3A4
MOTA	151	С	GLY	68	8.251	20.139	19.164	1.00	000	3A4
MOTA	152	0	GLY	68	8.314	18.954	18.839	1.00	0.00	3A4
ATOM	153	N	LYS	69	8.864	20.642	20.260	1.00	0.00	3A4 3A4
ATOM	154	CA	LYS	69	10.301	20.592	20.404	1.00	0.00	
ATOM	155	СВ	LYS	69	10.795	21.997	20.802	1.00	0.00	3A4
ATOM	156	CG	LYS	69	10.332	23.112	19.844	1.00	0.00	3A4 3A4
ATOM -	157	CD	LYS	69	10.770	24.527	20.225	1.00	0.00	3A4
ATOM	158	CE	LYS	69	9.876	25.161	21.300	1.00	0.00	3A4
ATOM	159	NZ	LYS	69	10.236	26.582	21.514	1.00	0.00	
ATOM	160	С	LYS	69	10.811	19.541	21.360	1.00	0.00	3A4 3A4
ATOM	161	0	LYS	69	11.914	19.033	21.177	1.00	0.00	3A4
ATOM	162	N	VAL	70	10.033	19.200	22.410	1.00	0.00	3A4
ATOM	163	CA	VAL	70	10.427	18.227	23.408	1.00	0.00	3A4
ATOM	164	СВ	VAL	70	10.984	18.837	24.696	1.00	0.00	3A4
ATOM	165		VAL	70	12.504	18.835	24.571	1.00	0.00	3A4
MOTA	166		VAL	70	10.344	20.206	25.037	1.00	0.00	3A4 3A4
MOTA	167	С	VAL	70	9.212	17.394	23.695	1.00	0.00	3A4
ATOM	168	0	VAL	70	8.176	17.901	24.111	1.00	0.00	3A4 3A4
MOTA	169	N	TRP	71	9.337	16.067	23.484	1.00	0.00	3A4 3A4
ATOM	170	CA	TRP	71	8.255	15.133	23.636		0.00	3A4 3A4
MOTA	171	CB	TRP	71	7.614	14.787	22.260			3A4
MOTA	172	CG	TRP	71	6.390	13.874	22.229			3A4
ATON	173	CD2	TRP	71	5.135	14.145	22.880	1.00	0.00	JAT

ATOM	174	CD1	TRP	71	6.251	12.660	21.615	1.00	0.00	3A4
ATOM	175		TRP	71	4.996	12.146	21.846	1.00	0.00	3A4 3A4
ATOM ATOM	176 177		TRP TRP	71 71	4.292 4.695	13.040 15.227	22.624 23.643	1.00	0.00	3A4
ATOM	178		TRP	71	2.995	12.995	23.131	1.00	0.00	3A4
ATOM	179		TRP	71	3.388	15.180	24.153	1.00	0.00	3A4
MOTA	180		TRP	71	2.551	14.080	23.902	1.00	0.00	3A4
ATOM	181	c o	TRP TRP	71 71	8.828 9.989	13.911 13.584	24.261 24.059	1.00	0.00	3A4 3A4
ATOM ATOM	182 183	N	GLY	72	7.987	13.188	25.027	1.00	0.00	3A4
ATOM	184	CA	GLY	72	8.345	11.936	25.647	1.00	0.00	3A4
MOTA	185	С	GLY	72	7.812	10.809	24.804	1.00	0.00	3A4
ATOM	186	0	GLY	72	6.679	10.850	24.336	1.00	0.00	3A4 3A4
ATOM ATOM	187 188	N CA	PHE	73 73	8.645 8.334	9.773 8.591	24.586 23.820	1.00	0.00	3A4
ATOM	189	СВ	PHE	73	9.278	8.443	22.586	1.00	0.00	3A4
ATOM	190	CG	PHE	73	8.893	7.320	21.647	1.00	0.00	3A4
ATOM	191		PHE	73	9.691	6.162	21.549	1.00	0.00	3A4
MOTA MOTA	192		PHE	73 73	7.717 9.320	7.398 5.105	20.877 20.707	1.00	0.00	3A4 3A4
ATOM	194		PHE	73	7.344	6.343	20.030	1.00	0.00	3A4
ATOM	195	CZ	PHE	73	8.146	5.196	19.947	1.00	0.00	3A4
MOTA	196	С	PHE	73	8.515	7.451	24.788	1.00	0.00	3A4
ATOM	197	0	PHE	73 74	9.257	7.543	25.757 24.540	1.00	0.00	3A4 3A4
MOTA MOTA	198 199	N CA	TYR TYR	74 74	7.826 7.884	6.328 5.174	25.397	1.00	0.00	3A4
ATOM	200	СВ	TYR	74	6.631	5.032	26.304	1.00	0.00	3A4
MOTA	201	CG	TYR	74	5.298	5.291	25.625	1.00	0.00	3A4
MOTA	202		TYR	74	4.515	4.223	25.146	1.00	0.00	3A4
MOTA MOTA	203 204		TYR TYR	74 74	4.797 3.279	6.603 4.456	25.491 24.524	1.00	0.00	3A4 3A4
ATOM	205	CE2	TYR	74	3.564	6.844	24.870	1.00	0.00	3A4
ATOM	206	CZ	TYR		2.804	5.769	24.384	1.00	0.00	3A4
ATOM	207	OH	TYR	74	1.560	6.006	23.757	1.00	0.00	3A4
ATOM ATOM	208 209	С 0	TYR TYR	74 74	8.100 7.256	4.007 3.682	24.486 23.658	1.00	0.00	3A4 · 3A4
ATOM	210	N	ASP	75	9.272	3.357	24.603	1.00	0.00	3A4
ATOM	211	CA	ASP	75	9.664	2.238	23.778	1.00	0.00	3A4
ATOM	212	СВ	ASP	75	11.110	2.479	23.220	1.00	0.00	3A4
ATOM ATOM	213 214	CG	ASP ASP	75 . 75 ·	11.483 10.755	1.556 1.577	22.044 21.015	1.00	0.00	3A4 3A4
ATOM	215		ASP	75	12.500	0.822	22.166	1.00	0.00	3A4
MOTA	216	С	ASP	75	9.580	1.007	24.657	1.00	0.00	3A4
MOTA	217	0	ASP	75	9.275	1.091	25.845	1.00	0.00	3A4
ATOM	218	N CA	GLY GLY	76 76	9.925 10.101	-0.191 -1.403	24.123 24.908	1.00	0.00	3A4 3A4
ATOM ATOM	219 220	CA	GLY	. 76	11.420	-1.335	25.643	1.00	0.00	3A4
ATOM	221	0	GLY	76	12.463	-1.562	25.039	1.00	0.00	3A4
MQTA	222	N	GLN	77	11.349	-0.928	26.946		.0.00	. 3A4
ATOM	223	CA	GLN	. 77 77	12.393	-0.521	27.882 27.835	1.00	0.00	3A4 3A4
ATOM ATOM	224 225	CB CG	GLN GLN	77	13.760 14.891	-1.300 -0.783	26.903	1.00	0.00	3A4
ATOM	226	CD	GLN	77	15.977	-1.843	26.760	1.00	0.00	3A4
ATOM	227	OE1		77	16.121	-2.718	27.611	1.00	0.00	3A4
ATOM	228	NE2		77	16.759	-1.765	25.648	1.00	0.00	3A4 3A4
ATOM ATOM	229 230	С 0	GLN GLN	77 77	12.593 12.935	0.983 1.504	27.782 26.719	1.00	0.00	3A4
ATOM	231	N	GLN	78	12.365	1.707	28.918	1.00	0.00	3A4
MOTA	232	CA	GLN	78	12.698	3.105	29.188	1.00	0.00	3A4
ATOM	233	СВ	GLN	78	14.220	3.411	28.944	1.00	0.00	3A4
ATOM ATOM	234 235	CG CD	GLN GLN	78 78	14.774 14.622	4.789 5.043	29.381 30.889	1.00	0.00	3A4 3A4
ATOM	236	OE1		78	14.409	4.138	31.694	1.00	0.00	3A4
MOTA	237	NE2	GLN	78	14.757	6.336	31.296	1.00	0.00	3A4
ATOM	238	C	GLN	78	11.820	4.135	28.453	1.00	0.00	3A4
MOTA MOTA	239 240	O N	GLN PRO	78 79	11.794 11.120	4.125 5.089	27.222 29.129	1.00	0.00	3A4 3A4
ATOM	241	CA	PRO	79	10.604	6.330	28.550	1.00	0.00	3A4
ATOM	242	CD	PRO	79	10.730	4.946	30.533	1.00	0.00	3A4
ATOM	243	CB	PRO	79 70	9.535	6.798	29.557	1.00	0.00	3A4
ATOM ATOM	244 245	CG C	PRO PRO	79 79	10.001 11.734	6.244	30.911	1.00	0.00	3A4 3A4

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ATOM	246	0	PRO	79	12.582	7.447	29.260	1.00	0.00	3A4
ATOM	247	N	VAL	80	11.782	8.012	27.228	1.00	0.00	3A4
MOTA	248	CA	VAL	80	12.870	8.876	26.835	1.00	0.00	3A4 3A4
MOTA	249	CB CG1	VAL	80 80	13.698 14.441	8.283 7.026	25.679 26.173	1.00	0.00	3A4
ATOM ATOM	250 251	CG2		80	12.828	7.028	24.440	1.00	0.00	3A4
ATOM	252	C	VAL	80	12.250	10.173	26.392	1.00	0.00	3A4
ATOM	253	0	VAL	80	11.117	10.204	25.939	1.00	0.00	3A4
MOTA	254	N	LEU	81	13.003	11.285	26.466	1.00	0.00	3A4
ATOM	255	CA	LEU	81	12.603	12.575 13.700	25.948 26.945	1.00	0.00	3A4 3A4
ATOM ATOM	256 257	CB CG	LEU	81 81	12.958 12.302	15.079	26.699	1.00	0.00	3A4
ATOM	258	CD1		81	10.822	15.078	27.116	1.00	0.00	3A4
MOTA	259	CD2		81	13.057	16.197	27.437	1.00	0.00	3A4
MOTA	260	C	LEU	81	13.352	12.751	24.647	1.00	0.00	3A4
MOTA	261	0	LEU	81	14.529	12.427	24.569 23.585	1.00	0.00	3A4 3A4
ATOM ATOM	262 263	N CA	ALA ALA	82 82	12.695 13.260	13.249 13.415	22.267	1.00	0.00	3A4
ATOM	264	CB	ALA	82	12.433	12.689	21.183	1.00	0.00	3A4
ATOM	265	c	ALA	82	13.288	14.890	21.990	1.00	0.00	3A4
MOTA	266	Ο.	ALA	82	12.251	15.546	22.002	1.00	0.00	3A4
MOTA	267	N	ILE	83	14.498	15.436	21.733	1.00	0.00	3A4 3A4
ATOM	268	CA CB	ILE	83 83	14.742 16.032	16.837 17.330	21.486 22.124	1.00	0.00	3A4
ATOM ATOM	269 270	CG2	ILE	83	15.944	18.846	22.217	1.00	0.00	3A4
ATOM	271	CG1		83	16.359	16.727	23.506	1.00	0.00	3A4
MOTA	272	CD	ILE	83	15.380	17.044	24.634	1.00	0.00	3A4
MOTA	273	C	ILE	83	14.831	17.000	19.986	1.00	0.00	3A4 3A4
ATOM	274	0	ILE	83 84	15.706 13.915	16.418 17.773	19.358 19.367	1.00	0.00	3A4
ATOM ATOM	275 276	N CA	THR THR	84	13.796	17.851	17.920	1.00	0.00	3A4
ATOM	277	СВ	THR	84	12.384	17.503	17.457	1.00	0.00	3A4
MOTA	278	OG1	THR	84	11.371	18.330	18.025	1.00	0.00	3A4
MOTA	279	CG2		84	12.085	16.027	17.808	1.00	0.00	3A4 3A4
ATOM	280	C	THR	84 84 -	14.259 14.500	19.175 19.282	17.344 16.144	1.00	0.00	3A4
ATOM ATOM	281 282	O N	THR ASP	84 - 85	14.371	20.231	18.176	1.00	0.00	3A4
ATOM	283	CA	ASP	85	14.595	21.594	17.732	1.00	0.00	3A4
ATOM	284	CB	ASP	85	13.703	22.550	18.577	1.00	0.00	3A4
ATOM	285	CG	ASP	85	13.371	23.873	17.872	1.00	0.00	3A4 3A4
ATOM ATOM	286 287	OD1		85 85	12.666 13.808	23.828 24.942	16.828 18.373	1.00	0.00	3A4
ATOM	288	C	ASP	85	16.050	21.928	17.888	1.00	0.00	3A4
ATOM	289	ō	ASP	85	16.660	21.452	18.843	1.00	0.00	3A4
ATOM	290	N	PRO	86	16.683	22.732	17.024	1.00	0.00	3A4
MOTA	291	CA	PRO	86	18.101 16.102	23.035	17.076 15.807	1.00	0.00	3A4 3A4
ATOM ATOM	292 293	CD CB	PRO PRO	86 86	18.421	23.257 23.751	15.747	1.00	0.00	3A4
ATOM	294	CG	PRO	86	17.079	24.309	15.294	1.00	0.00	3A4
MOTA	295	C	PRO	86	18.425	23.863	18.284	1.00	0.00	3A4
ATOM	296	0	PRO	86	19.466	23.647	18.892	1.00	0.00	3A4
ATOM	297	N	ASP	87 97	17.511 17.636	24.756 25.559	18.711 19.902	1.00	0.00	. 3A4 3A4
ATOM ATOM	298 299	CA CB	ASP ASP	87 87	16.417	26.494	20.029	1.00	0.00	3A4
ATOM	300	CG	ASP	87	16.305	27.442	18.820	1.00	0.00	3A4
ATOM	301		ASP	87	17.357	27.851	18.258	1.00	0.00	3A4
ATOM	302		ASP	87	15.148	27.764	18.439	1.00	0.00	3A4 3A4
ATOM ATOM	303 304	C O	ASP ASP	87 87	17.724 18.546	24.745 25.018	21.171 22.032	1.00	0.00	3A4
ATOM	305	N	MET	88	16.902	23.678	21.253	1.00	0.00	3A4
ATOM	306	CA	MET	88	16.847	22.776	22.375	1.00	0.00	3A4
ATOM	307	СВ	MET	88	15.536	22.000	22.396	1.00	0.00	3A4
ATOM	308	CG	MET	88	14.362	22.948	22.644	1.00	0.00	3A4 3A4
ATOM ATOM	309 310	SD CE	MET MET	88 88	12.947 13.722	22.177 21.914	23.469 25.087	1.00	0.00	3A4 3A4
ATOM	311	C	MET	88	18.007	21.812	22.436	1.00	0.00	3A4
ATOM	312	ŏ	MET	88	18.524	21.506	23.506	1.00	0.00	3A4
MOTA	313	N	ILE	89	18.500	21.349	21.264	1.00	0.00	3A4
ATOM	314	CA	ILE	89	19.637	20.450 19.800	21.170 19.793	1.00	0.00	3A4 3A4
MOTA MOTA	315 316	CB CG2	ILE ILE	89 89	19.679 21.088	19.800	19.793	1.00	0.00	3A4
ATOM	317		ILE	89	18.596	18.681	19.910	1.00	0.00	3A4

ATOM	318	CD	ILE	89	18.390	17.678	18.773	1.00	0.00		3A4
ATOM	319	С	ILE	89	20.916	21.161	21.538	1.00	0.00		3A4
MOTA	320	0	ILE	89	21.722	20.655	22.310	1.00	0.00		3A4
MOTA	321	N	LYS	90	21.096	22.421	21.089	1.00	0.00		3A4
MOTA	322	CA	LYS	90	22.214	23.250	21.481	1.00	0.00		3A4
MOTA	323	CB	LYS	90	22.225	24.577	20.719	1.00	0.00		3A4 3A4
MOTA	324	CG	LYS	90	23.531	25.387	20.790 19.811	1.00	0.00		3A4
MOTA	325	CD	LYS	90 90	23.546	26.569 27.339	19.774	1.00	0.00		3A4
ATOM	326 327	CE NZ	LYS LYS	90	25.167	27.975	21.082	1.00	0.00		3A4
MOTA MOTA	328	C	LYS	90	22.221	23.564	22.961	1.00	0.00		3A4
MOTA	329	ŏ	LYS	90	23.248	23.567	23.612	1.00	0.00		3A4
ATOM	330	N	THR	91	21.031	23.752	23.561	1.00	0.00		3A4
MOTA	331	CA	THR	91	20.855	23.981	24.981	1.00	0.00		3A4
ATOM	332	СВ	THR	91	19.434	24.380	25.293	1.00	0.00		3A4
ATOM	333	OG1	THR	91	19.170	25.637	24.681	1.00	0.00		3A4
ATOM	334	CG2	THR	91	19.109	24.554	26.810	1.00	0.00		3A4
ATOM	335	С	THR	91	21.198	22.782	25.817	1.00	0.00		3A4
ATOM	336	0	THR	91	21.850	22.889	26.851	1.00	0.00		3A4 3A4
ATOM	337	N	VAL	92	20.849	21.578	25.307	1.00	0.00		3A4
ATOM	338	CA	VAL	92	21.125	20.315 19.178	25.945 25.353	1.00	0.00		3A4
ATOM	339	CB	VAL VAL	92 92	21.025	18.247	24.370	1.00	0.00		3A4
MOTA	340 341		VAL	92	19.643	18.370	26.498	1.00	0.00		3A4
ATOM ATOM	342	C	VAL	92	22.600	20.047	26.089	1.00	0.00		3A4
ATOM	343	Ö	VAL	92	22.991	19.412	27.041	1.00	0.00		3A4
ATOM	344	N	LEU	93	23.483	20.706	25.311	1.00	0.00		3A4
ATOM	345	CA	LEU	93	24.914	20.851	25.543	1.00	0.00		3A4
ATOM	346	СВ	LEU	93	25.432	21.742	24.407	1.00	0.00		3A4
ATOM	347	CG	LEU	93	26.456	21.108	23.525	1.00	0.00		3A4
MOTA	348	CD1	LEU	93	25.796	19.892	22.820	1.00	0.00		3A4
ATOM	349	CD2	LEU	93	26.955	22.238	22.601	1.00	0.00		3A4
ATOM	350	С	LEU	93	25.419	21.473	26.847	1.00	0.00		3A4 3A4
ATOM	351	0	LEU	93	24.654	21.997	27.655	1.00	0.00		3A4
ATOM	352	N	VAL	94	26.774 27.599	21.385 21.729	27.035 28.196	1.00	0.00		3A4
ATOM	353	CA	VAL	94 94	27.328	23.082	28.879	1.00	0.00		3A4
ATOM ATOM	354 355	CB	VAL		28.368	23.358	30.001	1.00	0.00		3A4
ATOM	356		VAL	94	27.427	24.201	27.813	1.00	0.00		3A4
ATOM	357	c	VAL	94	27.515	20.540	29.137	1.00	0.00		3A4
ATOM	358	ŏ	VAL	94	26.875	20.578	30.188	1.00	0.00		3A4
ATOM	359	N	LYS	95	28.141	19.421	28.690	1.00	0.00		3A4
ATOM	360	CA	LYS	95	28.019	18.101	29,261	1.00	0.00		3A4
ATOM	361	CB	LYS	95	27.404	17.078	28.259	1.00	0.00		3A4
ATOM	362	CG	LYS	95	27.757	17.284	26.778	1.00	0.00		3A4
ATOM	363	CD	LYS	95	27.133	16.199	25.898	1.00	0.00		3A4 3A4
ATOM	364	CE	LYS	95	27.017 28.338	16.559	24.413 23.809	1.00	0.00		3A4
ATOM	365	NZ	LYS	95 95	29.379	16.819 17.675		1.00	0.00		3A4
ATOM	366	C O	LYS	95 95	30.123	16.990	29.040	1.00	0.00		3A4
ATOM ATOM	367 368	N	GLU	96	29.703	18.085	30.988	1.00	0.00		3A4
ATOM	369	CA	GLU	96	30.926	17.783	31.698	1.00	0.00	•	3A4
ATOM	370.	CB	GLU	96	31.795	19.051	31.950	1.00	0.00		3 <b>A</b> 4
ATOM	371		GLU	96	31.039	20.290	32.48,6	1.00			3A4
ATOM	372	CD	GLU	96	32.012	21.467	32.599	1.00	0.00		3A4
ATOM	373		GLU	96	31.790		31.901	1.00	0.00		3A4
MOTA	374	OE2	GLU	96	32.990	21.357	33.388	1.00	0.00		3A4
MOTA	375	С	GLU	96	30.517	17.078	32.969	1.00	0.00		3A4
MOTA	376	0	GLU	96	30.732	17.576	34.073	1.00	0.00		3A4 3A4
MOTA	377	И	CYS	97 02	29.924	15.869	32.763	1.00	0.00		3A4
ATOM	378	CA	CYS	97 97	29.436 29.558	14.865 15.141	33.693 35.235	1.00	0.00		3A4
MOTA	379 380	CB SG	CYS	97	29.186	13.706	36.313	1.00	0.00		3A4
ATOM ATOM	381	C	CYS	97	28.000	14.633	33.277	1.00	0.00		3A4
ATOM	382	õ	CYS	97	27.076	15.253	33.800	1.00	0.00		3A4
ATOM	383	N	TYR	98	27.817	13.703	32.305	1.00	0.00		3A4
ATOM	384	CA	TYR	98	26.556	13.216	31.782	1.00	0.00		3A4
ATOM	385	СВ	TYR	98	26.197	13.814	30.380	1.00	0.00		3A4
MOTA	386	CG	TYR	98	25.205	14.939	30.543	1.00	0.00		3A4
ATOM	387		TYR	98	25.573	16.198	31.050	1.00	0.00		3A4
MOTA	388		TYR		23.862	14.731	30.197	1.00	0.00		3A4
ATOM	389	CE1	TYR	98	24.626	17.224	31.198	1.00	0.00		3A4

ATOM	390	CE2	TYR	98	22.901	15.740	30.351	1.00	0.00		3A4
ATOM	391	CZ	TYR	98	23.286	16.993	30.849	1.00	0.00		3A4
ATOM	392	ОН	TYR	98	22.323	18.015	30.999	1.00	0.00		3A4
	393	c	TYR	98	26.800	11.735	31.683	1.00	0.00		3A4
ATOM	394	ō	TYR	98	27.629	11.292	30.891	1.00	0.00		3A4
ATOM				99	26.097	10.928	32.531	1.00	0.00		3A4
ATOM	395	N	SER				32.838	1.00	0.00		3A4
ATOM	396	CA	SER	99	26.414	9.536			0.00		3A4
ATOM	397	СВ	SER	99	25.870	9.141	34.247	1.00			3A4
ATOM	398	oG	SER	99	26.515	7.992	34.791	1.00	0.00		
ATOM	399	С	SER	99	25.931	8.568	31.771	1.00	0.00		3A4
MOTA	400	0	SER	99	24.885	8.764	31.156	1.00	0.00		3A4
MOTA	401	N	VAL	100	26.759	7.507	31.524	1.00	0.00		3A4
ATOM	402	CA	VAL	100	26.647	6.426	30.542	1.00	0.00		3A4
ATOM	403	CB	VAL	100	25.344	5.612	30.576	1.00	0.00		3A4
ATOM	404	CG1	VAL	100	25.483	4.356	29.677	1.00	0.00		3A4
ATOM	405	CG2	VAL	100	25.06 <b>2</b>	5.167	32.031	1.00	0.00		3A4
ATOM	406	C	VAL	100	26.977	6.962	29.152	1.00	0.00		3A4
ATOM	407	Ó	VAL	100	28.088	6.758	28.673	1.00	0.00		3A4
ATOM	408	N	PHE	101	26.002	7.682	28.517	1.00	0.00		3A4
ATOM	409	CA	PHE	101	26.131	8.581	27.372	1.00	0.00		3A4
ATOM	410	СВ	PHE	101	27.487	9.383	27.359	1.00	0.00		3A4
	411	CG	PHE	101	27.503	10.546	26.402	1.00	0.00		3A4
ATOM				101	26.587	11.609	26.522	1.00	0.00		3A4
ATOM	412		PHE			10.563	25.350	1.00	0.00		3A4
ATOM	413		PHE	101	28.432		25.573	1.00	0.00		3A4
ATOM	414		PHE	101	26.580	12.640		1.00	0.00		3A4
ATOM	415		PHE	101	28.435	11.597	24.418		0.00		3A4
MOTA	416	CZ	PHE	101	27.492	12.629	24.516	1.00			3A4
ATOM	417	С	PHE	101	25.860	7.863	26.049	1.00	0.00		3A4
ATOM	418	0	PHE	101	25.613	8.506	25.030	1.00	0.00		
ATOM	419	N	THR	102	25.881	6.507	26.048	1.00	0.00		3A4
ATOM	420	CA	THR	102	25.468	5.674	24.939	1.00	0.00		3A4
ATOM	421	CB	THR	102	26.561	5.456	23.875	1.00	0.00		3A4
ATOM	422	OG1	THR	102	26.134	4.618	22.803	1.00	0.00		3A4
ATOM	423	CG2	THR	102	27.920	4.971	24.441	1.00	0.00		3A4
ATOM	424	С	THR	102	24.949	4.448	25.660	1.00	0.00		3A4
ATOM	425	0	THR	102	25.680	3.511	25.976	1.00	0.00		3A4
ATOM	426	N	ASN	103	23.629	4.491	25.991	1.00	0.00		3A4
ATOM	427	CA	ASN	103	22.973	3.634	26.965	1.00	0.00		3A4
ATOM	428	СВ	ASN	103	22.145	4.482	28.000	1.00	0.00		3A4
ATOM	429	CG	ASN	103	21.193	5.519	27.373	1.00	0.00		3A4
ATOM	430		ASN	103	21.530	6.702	27.345	1.00	0.00		3A4
ATOM	431		ASN	103	19.993	5.093	26.893	1.00	0.00		3A4
ATOM	432	C	ASN	103	22.171	2.529	26.295	1.00	0.00		3A4
	433	ŏ	ASN	103	22.526	2.061	25.214	1.00	0.00		3A4
MOTA	434	N	ARG	104	21.099	2.084	27.018	1.00	0.00		3A4
ATOM				104	20.255	0.904	26.922	1.00	0.00		3A4
ATOM	435	CA	ARG		20.057	0.305	25.521	1.00	0.00		3A4
ATOM	436	CB	ARG	104		1.224	24.571	1.00	0.00		3A4
ATOM .	437	CG	ARG	104	19.266		23.096	1.00	0.00		3A4
ATOM	438	CD	ARG	104		. 0.794		1.00	0.00	•	3A4
ATOM	439	NE	ARG	104	20.722	1.001	22.589		0.00		3A4
MOTA	440	CZ	ARG	104	21.086	0.812	21.280	1.00	0.00		3A4
ATOM	441		ARG	104	22.383	1.027	20.912	1.00			3A4
ATOM	442		ARG	104	20.184	0.403	20.340	1.00	0.00		3A4
MOTA	443	С	ARG	104	20.801	-0.116	27.892	1.00	0.00		3A4
MOTA	444	0	ARG	104	21.996	~0.173	28.177	1.00	0.00		
MOTA	445	N	ARG	105	19.899	-0.953	28.439	1.00	0.00		3A4
ATOM	446	CA	ARG	105	20.180	-1.924	29.470	1.00	0.00		3A4
ATOM	447	СВ	ARG	105	18.917	-2.306	30.269	1.00	0.00		3A4
ATOM	448	CG	ARG	105	18.288	-1.109	31.012	1.00	0.00		3A4
MOTA	449	CD	ARG	105	17.273	-0.267	30.201	1.00	0.00		3A4
ATOM	450	NE	ARG	105	16.999	1.019	30.940	1.00	0.00		3A4
ATOM	451	CZ	ARG	105	17.736	2.168	30.769	1.00	0.00		3A4
ATOM	452		ARG	105	17.471	3.253	31.550	1.00	0.00		3A4
ATOM	453		ARG	105	18.734	2.262	29.841	1.00	0.00		3A4
ATOM	454	C	ARG	105	20.851	-3.183	28.984	1.00	0.00		3A4
MOTA	455	ō	ARG	105	21.862	-3.545	29.576	1.00	0.00		3A4
MOTA	456	N	PRO	106	20.439	-3.879	27.908	1.00	0.00		3A4
ATOM	457	CA	PRO	106	21.118	-5.066	27.409	1.00	0.00		3A4
	457	CD	PRO	106	19.166	-3.707	27.212	1.00	0.00		3A4
ATOM			PRO	106	20.292	-5.535	26.208	1.00	0.00		3A4
ATOM	459	CB			19.354	-4.383	25.861	1.00	0.00		3A4
MOTA	460	CG	PRO	106		-4.785	26.960	1.00	0.00		3A4
ATOM	461	С	PRO	106	22.531	-4.765	20.500	1.00	0.00		

ATOM	462	0	PRO	106	23.412	-5.580	27.239	1.00	0.00	3A4
ATOM	463	N ·	PHE	107	22.789	-3.612	26.347	1.00	0.00	3A4
MOTA	464	CA	PHE	107	24.092	-3.149	25.939	1.00	0.00	3A4
MOTA	465	СВ	PHE	107	23.996	-1.854	25.067	1.00	0.00	3A4
ATOM	466	CG	PHE	107		-2.185	23.730	1.00	0.00	3A4
ATOM	467		PHE	107	24.194	-2.404	22.604	1.00	0.00	· 3A4
ATOM	468		PHE	107	21.982	-2.301	23.578	1.00	0.00	3A4
ATOM	469		PHE	107	23.633	-2.730	21.360	1.00	0.00	3A4 3A4
MOTA	470		PHE	107 107	21.415 22.243	-2.640 -2.850	22.342	1.00	0.00	3A4
ATOM ATOM	471 472	CZ C	PHE PHE	107	24.996	-2.874	27.117	1.00	0.00	3A4
ATOM	473	ŏ	PHE	107	26.183	-3.178	27.071	1.00	0.00	3A4
ATOM	474	N	GLY	108	24.445	-2.352	28.235	1.00	0.00	3A4
ATOM	475	CA	GLY	108	25.169	-2.115	29.465	1.00	0.00	3A4
ATOM	476	С	GLY	108	25.703	-3.372	30.122	1.00	0.00	3A4
ATOM	477	0	GLY	108	26.825	-3.365	30.623	1.00	0.00	3A4
ATOM	478	N	PRO	109	24.957	-4.476	30.112	1.00	0.00	3A4
ATOM	479	CA	PRO	109	25.476	-5.825	30.348	1.00	0.00	3A4
ATOM	480	CD	PRO	109	24.065	-4.305	31.286	1.00	0.00	3A4
ATOM	481	СВ	PRO	109	24.191	-6.637	30.615	1.00	0.00	3A4 3A4
ATOM	482	CG	PRO	109 109	23.330 26.330	-5.658 -6.541	31.433 29.318	1.00	0.00	3A4
ATOM	483 484	C O	PRO PRO	109	27.456	-6.908	29.658	1.00	0.00	3A4
ATOM	485	N	VAL	110	25.774	-6.864	28.119	1.00	0.00	3A4
ATOM	486	CA	VAL	110	26.331	-7.778	27.133	1.00	0.00	3A4
ATOM	487	СВ	VAL	110	25.389	-8.936	26.768		0.00	3A4
ATOM	488		VAL	110	25.412	-9.943	27.938	1.00	0.00	3A4
ATOM	489	CG2	VAL	110	23.943	-8.492	26.450	1.00	0.00	3A4
ATOM	490	С	VAL	110	26.744	-6.971	25.923	1.00	0.00	3A4
MOTA	491	0	VAL	110	25.981	-6.165	25.392	1.00	0.00	3A4
ATOM	492	N	GLY	111	28.021	-7.174	25.497	1.00	0.00	3A4
ATOM	493	CA	GLY	111	28.732	-6.403	24.496	1.00	0.00	3A4 3A4
ATOM	494	C	GLY	111	29.773	-5.622 -4.588	25.245 25.839	1.00	0.00	3A4
ATOM	495 496	0	GLY	111 112	29.468 31.035	-6.136	25.266	1.00	0.00	3A4
ATOM ATOM	497	N CA	PHE	112	32.105	-5.711	26.158	1.00	0.00	3A4
ATOM	498	CB	PHE	112	32.907	-6.929	26.720	1.00	0.00	3A4
ATOM	499	CG	PHE	112	31.979	-7.800	27.529	1.00	0.00	3A4
ATOM	500		PHE	112	31.631	-9.095	27.096	1.00	0.00	3A4
ATOM	501		PHE	112	31.424	-7.318	28.732	1.00	0.00	3A4
ATOM	502	CE1	PHE	112	30.746	-9.883	27.847	1.00	0.00	3A4
MOTA	503	CE2	PHE	112	30.537	-8.104	29.480	1.00	0.00	3A4
ATOM	504	CZ	PHE	112	30.195	-9.387	29.035	1.00	0.00	3A4
ATOM	505	С	PHE	112	33.050	-4.749	25.472	1.00	0.00	3A4 3A4
ATOM	506	0	PHE	112	34.190 32.562	-5.078 -3.489	25.148 25.295	1.00	0.00	3A4
ATOM ATOM	507 508	N CA	MET MET	113 113	33.296	-2.314	24.869	1.00	0.00	3A4
ATOM	509	СВ	MET	113	32.602	-1.505	23.728	1.00	0.00	3A4
ATOM	510	CG	MET	113	32.554	-2.210	22.356	1.00	0.00	3A4
ATOM	511	SD	MET	113	31.429	-3.639	22.184	1.00	0.00	3A4
ATOM	512	CE	MET	113	29.851	-2.787	22.471	1.00	0.00	3A4
ATOM	513	С	MET	113	33.386	-1.481	26.125	1.00	0.00	3A4
ATOM	514	0	MET	113	32.371	-1.027	26.652	1.00	0.00	3A4
MOTA	515	N	LYS	114	•	-1.321	26.660	1.00	0.00	3A4
ATOM	516	CA	LYS	114	34.932	-0.910	28.025	1.00	0.00	3A4
ATOM	517	CB	LYS	114	36.207	-1.643	28.544	1.00	0.00	3A4 3A4
ATOM	518	CG	LYS	114	36.129	-3.170 -3.890	28.392 28.832	1.00	0.00	3A4
ATOM	519	CD	LYS	114	37.411	-5.417	28.667	1.00	0.00	3A4
ATOM ATOM	520 521	CE NZ	LYS LYS	114 114	37.355 37.190	-5.806	27.244	1.00	0.00	3A4
ATOM	522	C	LYS	114	35.074	0.600	28.136	1.00	0.00	3A4
ATOM	523	ŏ	LYS	114	34.485	1.339	27.348	1.00	0.00	3A4
ATOM	524	N	SER	115	35.857	1.092	29.141	1.00	0.00	3A4
ATOM	525	ÇA	SER	115	35.955	2.486	29.566	1.00	0.00	3A4
MOTA	526	СВ	SER	115	36.419	2.597	31.048	1.00	0.00	3A4
MOTA	527	OG	SER	115	35.505	1.921	31.901	1.00	0.00	3A4
MOTA	528	С	SER	115	36.891	3.307	28.696	1.00	0.00	3A4
ATOM	529	0	SER	115	38.106	3.302	28.890	1.00	0.00	3A4 3A4
ATOM	530	N	ALA	116	36.300	4.041	27.709 26.770	1.00	0.00	3A4 3A4
ATOM	531 532	CA CB	ALA ALA	116 116	36.990 36.806	4.440	25.323	1.00	0.00	3A4
ATOM ATOM	532	CB	ALA	116	36.445		26.942	1.00	0.00	3A4
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ATOM	534	0	ALA	116	35.934	6.634	27.995		0.00	3A4
ATOM	535	N	ILE	117	36.498	7.116	25.886		0.00	3A4
ATOM	536	CA	ILE	117	36.054	8.497	25.985		0.00 0.00	3A4 3A4
ATOM	537	CB	ILE	117	36.818 36.637	9.363 8.922	24.999 23.524	_	0.00	3A4
ATOM	538	CG2	ILE	117 117	36.647	10.857	25.212		0.00	3A4
ATOM ATOM	539 540	CD	ILE	117		11.262	26.574		0.00	3A4
ATOM	541	c	ILE	117	34.556	8.659	25.822		0.00	3A4
ATOM	542	0	ILE	117	33.924	9.474	26.492		0.00	3A4
MOTA	543	N .	SER	118	33.923	7.843	24.946	1.00	0.00	3A4 3A4
MOTA	544	CA	SER	118	32.533 32.205	8.033 7.525	24.588 23.146	1.00	0.00	3A4
ATOM	545 546	CB OG	SER SER	118 118	32.499	6.147	22.946	1.00	0.00	3A4
MOTA MOTA	547	C		118	31.585	7.455	25.606	1.00	0.00	3A4
ATOM	548	ō	SER	118	30.395	7.686	25.524	1.00	0.00	3A4
ATOM	549	N	ILE	119	32.084	6.735	26.630	1.00	0.00	3A4 3A4
MOTA	550	CA	ILE	119	31.251	6.157	27.657 27.705	1.00	0.00	3A4
ATOM	551	CB	ILE	119 119	31.480 32.895	4.637 4.296	28.225	1.00	0.00	3A4
MOTA MOTA	552 553		ILE	119	30.373	3.794	28.400	1.00	0.00	3A4
ATOM	554	CD	ILE	119	29.071	3.681	27.605	1.00	0.00	3A4
ATOM	555	ç	ILE	119	31.475	6.827	29.005	1.00	0.00	3A4
ATOM	556	0	ILE	119	30.894	6.426	30.013	1.00	0.00	3A4 3A4
ATOM	557	N	ALA	120	32.350	7.862	29.050 30.276	1.00	0.00	3A4
ATOM	558	CA	ALA	120	32.876 34.429	8.420 8.417	30.275	1.00	0.00	3A4
ATOM	559 560	CB C	ALA ALA	120 120	32.403	9.821	30.537	1.00	0.00	3A4
ATOM ATOM	561	0	ALA	120	32.153	10.624	29.642	1.00	0.00	3A4
ATOM	562	N	GLU	121	32.338	10.132	31.847	1.00	0.00	3A4
MOTA	563	CA	GLU	121	31.987	11.402	32.421	1.00	0.00	3A4 3A4
ATOM	564	CB	GLU	121	31.189	11.213	33.742 33.613	1.00 1.00	0.00	3A4
ATOM	565	CG	GLU	121 121	29.884 30.124	8.902	33.618	1.00	0.00	3A4
ATOM ATOM	566 567	CD OE1	GLU	121	29.800	8.241	32.594	1.00	0.00	3A4
ATOM	568		GLU	121	30.631	8.385	34.649	1.00	0.00	3A4
ATOM	569	С	GLU	121	33.282	12.104	32.738	1.00	0.00	3A4 3A4
ATOM	570	0	GLU	121	34.307	11.460	32.947	1.00	0.00	3A4 3A4
ATOM	571	N	ASP	122	33.267 34.366	13.450 14.255	32.868 33.384	1.00	0.00	3A4
ATOM	572 573	CA CB	ASP ASP	122 122	33.940	15.762	33.320	1.00	0.00	3A4
ATOM ATOM	574	CG	ASP	122	35.057	16.786	33.606	1.00	0.00	3A4
ATOM	575		ASP	122	34.911	17.556	34.593	1.00	0.00	3A4
MOTA	576		ASP	122	36.057	16.817	32.842	1.00	0.00	3A4 3A4
ATOM	577	C	ASP	122	34.615 33.636	13.879 13.610	34.870 35.566	1.00	0.00	3A4
MOTA	578 579	O N	ASP GLU	122 123	35.863	13.792	35.421	1.00	0.00	3A4
ATOM ATOM	580	CA	GLU	123	37.162	14.248	34.972	1.00	0.00	3A4
ATOM	581	СВ	GLU	123	37.993	14.687	36.197	1.00	0.00	3A4
ATOM	582	CG	GLU	123	37.348	15.854	36.968		0.00	3A4 3A4
MOTA	583	CD	GLU	123	38.253	16.265 17.417	38.134 38.116	1.00	0.00	3A4
ATOM	584		GLU	123 123	38.764 38.443	15.431	39.060	1.00	0.00	3A4
ATOM ATOM	585 586	C	GLU	123	37.950	13.205	34.211	1.00	0.00	3A4
ATOM	587	ŏ	GLU	123	39.000	13.494	33.638	1.00	0.00	3A4
ATOM	588	N	GLU	124	37.449	11.951	34.149	1.00	0.00	3A4 3A4
ATOM	589	CA	GLU	124	38.063	10.827	33.460 33.756	1.00	0.00	3A4
MOTA	590	CB	GLU GLU	124 124	37.284 37.186	9.523 9.213	35.261	1.00	0.00	3A4
MOTA MOTA	591 592	CG CD	GLU		36.410	7.908	35.465		0.00	3A4
MOTA	593		L GLU		37.010	6.933	35.993	1.00		3A4
ATOM	594		2 GLU		35.204	7.870			_	3A4 3A4
MOTA	595	С	GLU		38.109	11.000				3A4
ATOM	596	0	GLU		39.087 37.027	10.727 11.579				3A4
ATOM	597	N	TRP TRP		36.896	11.901				3A4
MOTA MOTA	598 599	CA CB	TRP		35.456	12.317			0.00	3A4
ATOM	600	CG			35.096	13.136				3A4
ATOM	601		2 TRP		34.736	14.501				3A4 3A4
ATOM	602		1 TRP		34.423	12.765 13.815				3A4
ATOM	603		1 TRP 2 TRP		33.701 33.805	14.860				3A4
ATOM ATOM	604 605		2 TRP		35.040	15.361				3A4
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ATOM	606	CZ2	TRP	125	33.124	16.059	27.921	1.00	0.00	3A4
ATOM	607		TRP	125	34.396	16.599	29.921	1.00	0.00	3A4
ATOM	608		TRP	125	33.421	16.924	28.984 29.585	1.00	0.00	3A4 3A4
MOTA	609 610	С О	TRP TRP	125 125	37.893 38.564	12.940 12.734	28.590	1.00	0.00	3A4
MOTA MOTA	611	N	LYS	126	38.066	14.068	30.315	1.00	0.00	3A4
ATOM	612	CA	LYS	126	38.948	15.161	29.915	1.00	0.00	3A4
ATOM	613	СВ	LYS	126	38.776	16.362	30.855	1.00	0.00	3A4
MOTA	614	CG	LYS	126	39.424	17.682	30.406	1.00	0.00	3A4
ATOM	615	CD	LYS	126	39.026	18.858	31.300	1.00 1.00	0.00	3A4 3A4
ATOM	616	CE NZ	LYS LYS	126 126	39.634 39.206	20.191 21.296	30.845 31.735	1.00	0.00	. 3A4
ATOM ATOM	617 618	C	LYS	126	40.413	14.775	29.867	1.00	0.00	3A4
ATOM	619	ŏ	LYS	126	41.152	15.173	28.977	1.00	0.00	3A4
ATOM	620	N	ARG	127	40.830	13.884	30.785	1.00	000	3A4
ATOM	621	CA	ARG	127	42.152	13.315	30.821	1.00	0.00	3A4 3A4
ATOM	622	CB	ARG	127	42.369	12.556	32.148 33.385	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	623 624	CG CD	ARG ARG	127 127	42.319 42.230	13.460 12.652	34.686	1.00	0.00	3A4
ATOM	625	NE	ARG	127	42.079	13.613	35.835	1.00	0.00	3A4
ATOM	626	CZ	ARG	127	41.521	13.267	37.040	1.00	0.00	3A4
MOTA	627	NH1	ARG	127	41.438	14.206	38.026	1.00	0.00	3A4
ATOM .	628		ARG	127	41.040	12.009	37.276	1.00	0.00	3A4 3A4
ATOM	629	C	ARG	127	42.448	12.378 12.464	29.678 29.060	1.00	0.00	3A4
ATOM ATOM	630 631	O N	ARG	127 128	43.503 41.487	11.489	29.329	1.00	0.00	3A4
ATOM	632	CA	LEU	128	41.614	10.553	28.227	1.00	0.00	3A4
ATOM	633	СВ	LEU	128	40.552	9.436	28.305	1.00	0.00	3A4
MOTA	634	CG	LEU	128	40.710	8.475	29.510	1.00	0.00	3A4
ATOM	635		LEU	128	39.492	7.536	29.620	1.00	0.00	3A4 3A4
ATOM	636		LEU	128 128	42.026 41.513	7.670 11.260	29.503 26.900	1.00	0.00	3A4
MOTA MOTA	637 638	C O	LEU	128	42.307	10.998	26.016	1.00	0.00	3A4
ATOM	639	N	λRG	129	40.613	12.256	26.764	1.00	0.00	3A4
ATOM	640	CA	ARG	129	40.455	13.056	25.570	1.00	0.00	3A4
MOTA	641	CB	ARG	129	39.248	13.995	25.706	1.00	0.00	3A4
MOTA	642	CG	ARG	129	38.865	14.698 15.285	24.411 24.477	1.00	0.00	3A4 3A4
ATOM ATOM	643 644	CD NE	ARG	129 129	37.443 36.965	15.632	23.089	1.00	0.00	3A4
ATOM	645	CZ	ARG	129	37.094	16.870	22.512	1.00	0.00	3A4
ATOM	646		ARG	129	36.589	17.069	21.260	1.00	0.00	3A4
MOTA	647		ARG	129	37.709	17.907	23.155	1.00	0.00	3A4
ATOM	648	C	ARG	129	41.673	13.896	25.247	1.00	0.00	3A4 3A4
ATOM	649	O N	ARG SER	129 130	42.125 42.292	13.963 14.491	24.109 26.294	1.00	0.00	3A4
ATOM ATOM	650 651	CA	SER	130	43.486	15.299	26.191	1.00	0.00	3A4
ATOM	652	СВ	SER	130	43.870	16.030	27.515	1.00	0.00	3A4
MOTA	653	OG	SER	130	42.925	17.049	27.812	1.00	0.00	3A4
MOTA	654	С	ŞER	130	44.691	14.547	25.703	1.00	0.00	3 <u>4</u> 4 3A4
MOTA	655	0	SER	130 131	45.506 44.822	15.121 · 13.241	25.002 26.004	1.00	0.00	3A4
ATOM ATOM	656 657	N CA	LEU	131	45.894	12.396	25.508	1.00	0.00	3A4
ATOM	658	CB	LEU	131	45.835	11.013	26.195	1.00	0.00	3A4
MOTA	659		LEU	131	46.473	11.008	27.591		0.00	3A4
ATOM	660		LEU	131	45.836	9.924	28.474	1.00	0.00	3A4
ATOM	661		LEU	131	48.005	10.845 12.189	27.482 24.006	1.00	0.00	3A4 3A4
ATOM ATOM	662 663	С 0	LEU	131 131	45.875 46.913	12.177	23.361	1.00	0.00	3A4
ATOM	664	Ŋ	LEU	132	44.675	12.059	23.421	1.00	0.00	3A4
ATOM	665	CA	LEU	132	44.436	11.692	22.040	1.00	0.00	3A4
MOTA	666	CB	LEU	132	43.113	10.883	21.884	1.00	0.00	3A4
ATOM	667	CG	LEU	132	42.628 41.170	10.220 9.739	23.187 23.225	1.00	0.00	3A4 3A4
ATOM ATOM	668 669		LEU	132 132	43.579	9.147	23.759	1.00	0.00	3A4
ATOM	670	C	LEU	132	44.339	12.896	21.142	1.00	0.00	3A4
ATOM	671	ō	LEU	132	44.709	12.862	19.975	1.00	0.00	3A4
ATOM	672	N	SER		43.808	14.009	21.685	1.00	0.00	3A4
MOTA	673	CA	SER		43.570	15.239	20.967	1.00	0.00	3A4 3A4
MOTA	674 675	CB OG	SER		42.882 43.525	16.277 16.664	21.854 23.058	1.00	0.00	3A4
MOTA MOTA	676	C	SER		44.766	15.878	20.280	1.00	0.00	3A4
ATOM	677	ŏ	SER		44.586	16.429	19.192	1.00	0.00	3A4

ATOM	678	N	PRO	134	46.017	15.798	20.777	1.00	0.00	3A4
ATOM	679	CA	PRO	134	47.159	16.327	20.076	1.00	0.00	3A4
MOTA	680	ÇD	PRO	134	46.405	15.537	22.155	1.00	0.00	3A4
ATOM	681	СВ	PRO	134	48.327	16.318	21.087	1.00	0.00	3A4
MOTA	682	CG	PRO	134	47.635	16.387	22.434	1.00	0.00	3A4 3A4
MOTA	683	C	PRO	134	47.567 48.106	15.563 16.175	18.844 17.927	1.00	0.00	3A4
ATOM	684	О И	PRO THR	134 135	47.305	14.235	18.803	1.00	0.00	3A4
ATOM ATOM	685 686	CA	THR	135	47.657	13.342	17.727	1.00	0.00	3A4
ATOM	687	СВ	THR	135	47.864	11.912	18.232	1.00	0.00	3A4
ATOM	688		THR	135	46.681	11.299	18.729	1.00	0.00	3A4
ATOM	689	CG2	THR	135	48.889	11.953	19.387	1.00	0.00	3A4
ATOM	690	С	THR	135	46.639	13.419	16.594	1.00	0.00	3A4
ATOM	691	0	THR	135	46.921	13.057	15.460	1.00	0.00	3A4 3A4
ATOM	692	N	PHE	136	45.420	13.916 13.979	16.895 15.962	1.00	0.00	3A4
ATOM	693	CA CB	PHE	136 136	44.322 43.007	13.434	16.581	1.00	0.00	3A4
ATOM ATOM	694 695	CG	PHE	136	43.069	12.028	17.109	1.00	0.00	3A4
ATOM	696		PHE	136	42.397	11.733	18.297	1.00	0.00	3A4
ATOM	697		PHE	136	43.793	10.992	16.495	1.00	0.00	3A4
ATOM	698	CEl	PHE	136	42.237	10.417	18.717	1.00	0.00	3A4
ATOM	699	CE2	PHE	136	43.668	9.665	16.926	1.00	0.00	3A4
MOTA	700	CZ	PHE	136	42.847	9.372	18.017	1.00	0.00	3A4 3A4
MOTA	701	C	PHE	136	44.074	15.402 15.703	15.465	1.00	0.00	3A4
ATOM	702	0	PHE	136	42.971 45.088	16.323	15.025 15.493	1.00	0.00	3A4
ATOM	703 704	N CA	THR	137 137	44.944	17.764	15.224	1.00	0.00	3A4
MOTA MOTA	705	CB	THR	137	46.098	18.572	15.830	1.00	0.00	3A4
ATOM	706		THR	137	46.156	18.321	17.228	1.00	0.00	3A4
ATOM	707		THR	137	45.936	20.108	15.640	1.00	0.00	3A4
MOTA	708	С	THR	137	44.796	18.094	13.739	1.00	0.00	3A4
ATOM	709	0	THR	137	43.885	18.830	13.359	1.00	0.00	3A4
ATOM	710	N	SER	138	45.685	17.534	12.870 11.419	1.00	0.00	3A4 3A4
ATOM	711	CA	SER	138	45.656 47.076	17.677 17.874	10.806	1.00	0.00	3A4
ATOM ATOM	712 713	CB OG	SER	138 138	47.648	19.086	11.280	1.00	0.00	3A4
ATOM	714	c	SER	138	45.012	16.431	10.860	1.00	0.00	3A4
ATOM	715	ō	SER	138	43.868	16.450	10.408	1.00	0.00	3A4
ATOM	716	N	GLY	139	45.756	15.304	10.953	1.00	0.00	3A4
ATOM	717	CA	GLY	139	45.288	13.957	10.734	1.00	0.00	3A4
ATOM	718	С	GLY	139	45.698	13.207	11.960	1.00	0.00	3A4
ATOM	719	0	GLY	139	46.061	13.818 11.847	12.961 11.918	1.00	0.00 0.00	3A4 3A4
ATOM	720 721	N CA	LYS LYS	140 140	45.629 45.777	10.945	13.054	1.00	0.00	3A4
ATOM ATOM	722	CB	LYS	140	44.729	9.786	13.048	1.00	0.00	3A4
ATOM	723	CG	LYS	140	43.246	10.097	13.336	1.00	0.00	3A4
ATOM	724	CD	LYS	140	42.846	11.560	13.252	1.00	0.00	3A4
MOTA	725	CE	LYS	140	41.456	11.872	13.770	1.00	0.00	3A4
MOTA	726	NZ	LYS	140	41.193	13.331	13.606	1.00	0.00	. 3A4 3A4
ATOM	727	C	LYS	140	47.165	10.340 9.123	13.065 12.976	1.00	0.00	3A4
ATOM	728 729	O N	LYS LEU	140 141	47.330 48.195	11.212	13.185	1.00	0.00	3A4
ATOM ATOM	730	CA	LEU	141	49.585	10.835	13.207	1.00	0.00	3A4
ATOM	731	СВ	LEU	141	50.096	10.321	11.825	1.00	0.00	3A4
ATOM	732	CG	LEU	141	51.411	9.530	11.812	1.00	0.00	3A4
MOTA	733	CD1	LEU	141	52.059	9.603	10.425	1.00	0.00	3A4
ATOM	734		LEU	141	51.161	8.066	12.211	1.00	0.00	3A4
ATOM	735	С	LEU	141	50.286	12.100	13.623	1.00	0.00	3A4 3A4
ATOM	736	0	LEU	141	50.455 50.687	12.362 12.924	14.813 12.618	1.00	0.00	3A4
ATOM ATOM	737 738	N CA	LYS	142 142	51.307	14.222	12.760	1.00	0.00	3A4
ATOM	739	СВ	LYS		52.868	14.192	12.729	1.00	0.00	3A4
ATOM	740	CG	LYS		53.516	13.465	13.915	1.00	0.00	3A4
ATOM	741	CD	LYS		55.045	13.555	13.916	1.00	0.00	3A4
ATOM	742	CE	LY\$		55.714	12.858	15.108	1.00	0.00	3A4
MOTA	743	NZ	LYS		55.454	11.401	15.086	1.00	0.00	3A4
MOTA	744	C	LYS		50.813	15.068	11.606 11.736	1.00	0.00	3A4 3A4
ATOM	745	0	LYS		50.704 50.529	16.287 14.432	10.433	1.00	0.00	3A4
ATOM ATOM	746 747	N CA	GLU GLU		50.169	15.105	9.198	1.00	0.00	3A4
ATOM	747	CB	GLU		51.389	15.242	8.234	1.00	0.00	3A4
ATOM	749	CG	GLU		51.158	16.046	6.935	1.00	0.00	3A4
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ATOM	750	CD	GLU	143	50.774	17.493	7.267	_	0.00	3A4
ATOM	751	OE1		143	51.602	18.194	7.909		0.00	3A4
ATOM	752	OE2	GLU	143	49.651	17.917	6.882	_	0.00	3A4 3A4
ATOM	753		GLU	143	49.047	14.324	8.559	1.00	0.00 0.00	3A4
ATOM	754		GLU	143	47.898	14.760 13.160	8.605 7.926		0.00	3A4
ATOM	755		MET	144	49.393 48.584	12.130	7.300	1.00	0.00	3A4
MOTA	756		MET MET	144 144	47.303	11.759	8.070	1.00	0.00	3A4
ATOM ATOM	757 758	CG	MET	144	47.567	10.932	9.334	1.00	0.00	3A4
ATOM	759	SD	MET	144	48.269	9.267	9.019	1.00	0.00	3A4
ATOM	760	CE	MET	144	47.029	8.504	7.928	1.00	0.00	3A4
ATOM	761	С	MET	144	48.192	12.409	5.879	1.00	0.00	3A4
ATOM	762	0	MET	144	47.891	11.472	5.150	1.00	0.00	3A4 3A4
MOTA	763	N	VAL	145	48.169	13.678	5.428 4.130	1.00	0.00	3A4
ATOM	764	CA	VAL	145	47.650 47.693	14.088 15.597	3.949	1.00	0.00	3A4
MOTA	765	CB	VAL VAL	145 145	46.839	16.061	2.734	1.00	0.00	3A4
ATOM ATOM	766 767		VAL	145	47.128	16.245	5.237	1.00	0.00	3A4
ATOM	768	C	VAL	145	48.261	13.425	2.906	1.00	0.00	3A4
ATOM	769	ŏ	VAL	145	47.501	13.014	2.026	1.00	0.00	3A4
ATOM	770	N	PRO	146	49.595	13.235	2.821	1.00	0.00	3A4
ATOM	771	CA	PRO	146	50.226	12.490	1.741	1.00	0.00	3A4 3A4
MOTA	772	CD	PRO	146	50.623	13.942	3.599	1.00	0.00	3A4 3A4
MOTA	773	CB	PRO	146	51.743	12.625	1.988	1.00	0.00	3A4
ATOM	774	CG	PRO	146	51.872	13.954 11.029	2.721 1.698	1.00	0.00	3A4
ATOM	775	C	PRO	146 146	49.826 49.678	10.483	0.613	1.00	0.00	3A4
ATOM	776 777	O N	PRO ILE	147	49.572	10.388	2.863	1.00	0.00	3A4
ATOM ATOM	778	CA	ILE	147	49.098	9.027	2.976	1.00	0.00	3A4
ATOM	779	СВ	ILE	147	49.254	8.469	4.382	1.00	0.00	3A4
ATOM	780		ILE	147	48.993	6.930	4.422	1.00	0.00	3A4
MOTA	781	CG1	ILE	147	50.685	8.809	4.901	1.00	0.00	3A4 3A4
MOTA	782	CD	ILE	147	51.018	8.281	6.300 2.564	1.00	0.00	3A4
MOTA	783	С	ILE	147	47.660	8.881 7.899	1.922	1.00	0.00	3A4
ATOM	784	0	ILE	147 148	47.306 46.789	9.866	2.875	1.00	0.00	3A4
ATOM	785 786	N CA	ILE	148	45.386	9.833	2.503	1.00	0.00	3A4
ATOM ATOM	787	CB	ILE	148	44.570	10.932	3.172	1.00	0.00	3A4.
ATOM	788	CG2		148	43.057	10.768	2.811	1.00	0.00	3A4
ATOM	789	CG1		148	44.675	10.809	4.718	1.00	0.00	3A4
MOTA	790	CD	ILE	148	44.158	12.030	5.488	1.00	0.00	3A4 3A4
MOTA	791	C	ILE	148	45.218	9.888	1.005	1.00	0.00	3A4
ATOM	792	0	ILE	148	44.486 46.000	9.106 10.765	0.350	1.00	0.00	3A4
MOTA	793 794	N CA	ALA ALA	149 149	46.058	10.923	-1.086	1.00	0.00	3A4
ATOM ATOM	795	CB	ALA	149	46.983	12.097	-1.414	1.00	0.00	3A4
ATOM	796	c	ALA	149	46.539	9.682	-1.803	1.00	0.00	3A4
ATOM	797	0	ALA	149	45.965	9.246	-2.797	1.00	0.00	· 3A4
MOTA	798	N	GLN	150	47.578	9.019	-1.243	1.00	0.00	3A4 3A4
ATOM	799	CA	GLN	150	48.121	7.780	-1.753	1.00	0.00	· 3A4
MOTA	800	CB	GLN	150	49.342 50.637	7.295 8.037	-0.954 -1.297	1.00	0.00	3A4
MOTA	801	CG	GLN GLN	150 150	51.737	7.586	-0.326	1.00	0.00	3A4
ATOM	802 803	CD	GLN	150	52.080	6.406	-0.292	1.00	0.00	3A4
ATOM ATOM	804		GLN	150	52.300	8.525	0.483	1.00	0.00	3A4
ATOM	805	c	GLN	150	47.129	6.663	-1.774	1.00	0.00	3A4
MOTA	806	0	GLN	150	46.962	5.992	-2.789	1.00	0.00	3A4 3A4
MOTA	807	N	TYR		46.371	6.500	-0.658	1.00	0.00	3A4
ATOM	808	CA	TYR		45.418	5.431	-0.538 0.859		0.00	3A4
ATOM	809	CB	TYR		44.853 44.181	5.227 3.823	0.880			3A4
MOTA	810	CG	TYR		43.188	3.417	1.745			3A4
ATOM ATOM	811 812		TYR TYR		44.795	2.750	0.124			3A4
ATOM	813		TYR		42.443	2.274	1.345			3A4
ATOM	814		TYR		44.170	1.533	-0.113			3A4
ATOM	815	CZ	TYR	151	42.935	1.315	0.454			3A4 3A4
ATOM	816	OH	TYR		42.254	0.104	0.201			3A4
MOTA	817	С	TYP		44.221	5.669	-1.449 -2.103			3A4 3A4
ATOM	818	0	TYR		43.738 43.775	4.750 6.936	-2.103			3A4
MOTA	819	N CA	GLY GLY		42.703	7.368	-2.423			3A4
MOTA MOTA	820 821	CA	GLY		42.962	7.025	-3.877			3A4
WY OU	251	-				_				

MOTA	822	0	GLY	152	42.122	6.466	-4.565	1.00	0.00	3A4
ATOM	823	N	ASP	153	44.194	7.284	~4.339	1.00	0.00	3A4
ATOM	824	CA	ASP	153	44.647	6.996	-5.674	1.00	0.00	3A4
ATOM	825	CB	ASP	153	46.061	7.586	-5.844	1.00	0.00	3A4
ATOM	826	CG	ASP	153	45.993	9.119	-5.945	1.00	0.00	3A4
ATOM	827	ODl		153	45.014	9.650	-6.534	1.00	0.00	3A4 3A4
ATOM	828	OD2		153	46.922	9.784	-5.416	1.00	0.00	3A4 3A4
ATOM	829	С	ASP	153	44.703	5.521	-6.007	1.00	0.00	3A4
MOTA	830	0	ASP	153	44.288	5.096	-7.076	1.00	0.00	3A4
ATOM	831	N	VAL	154	45.154	4.686	-5.048 -5.160	1.00	0.00	3A4
ATOM	832	CA	VAL	154	45.173 45.878	3.235 2.605	-3.160	1.00	0.00	3A4
ATOM	833 834	CB	VAL VAL	154 154	45.770	1.054	-3.875	1.00	0.00	3A4
ATOM ATOM	835		VAL	154	47.373	2.989	-4.067	1.00	0.00	3A4
ATOM	836	C	VAL	154	43.793	2.651	-5.283	1.00	0.00	3A4
ATOM	837	ŏ	VAL	154	43.531	1.783	-6.112	1.00	0.00	3A4
ATOM	838	N	LEU	155	42.842	3.184	-4.494	1.00	0.00	3A4
ATOM	839	CA	LEU	155	41.460	2.758	-4.505	1.00	0.00	3A4
ATOM	840	СB	LEU	155	40.697	3.480	-3.395	1.00	0.00	3A4
ATOM	841	CG	LEU	155	41.005	3.018	-1.989	1.00	0.00	3A4
ATOM	842	CD1	LEU	155	40.785	4.226	-1.096	1.00	0.00	3A4
ATOM	843	CD2	LEU	155	40.117	1.825	-1.591	1.00	0.00	3A4
ATOM	844	С	LEU	155	40.732	3.082	-5.782	1.00	0.00	3A4
ATOM	845	0	LEU	155	39.955	2.295	-6.313	1.00	0.00	3A4 3A4
ATOM	846	N	VAL	156	41.020	4.276	-6.333	1.00	0.00	3A4
ATOM	847	CA	VAL	156	40.441	4.744 6.216	-7.564 -7.769	1.00	0.00	3A4
ATOM	848	СВ	VAL	156	40.709	6.709	-9.147	1.00	0.00	3A4
ATOM	849		VAL	156	40.208 39.887	6.989	-6.709	1.00	0.00	- 3A4
ATOM	850 851	CGZ	VAL VAL	156 156	40.956	3.916	-8.726	1.00	0.00	3A4
MOTA MOTA	852	0	VAL	156	40.186	3.474	-9.566	1.00	0.00	3A4
ATOM	853	N	ARG	157	42.263	3.571	-8.714	1.00	0.00	3A4
ATOM	854	CA	ARG	157	42.881	2.692	-9.687	1.00	0.00	3A4
ATOM	855	СВ	ARG	157	44.400	2.603	-9.480	1.00	0.00	3A4
ATOM	856	CG	ARG	157	45.201		-10.646	1.00	0.00	3A4
MOTA	857	CD	ARG	157	46.718		-10.406	1.00	0.00	3A4
ATOM	858	NE	ARG	157	47.008	0.982	-9.282	1.00	0.00	3A4
MOTA	859	CZ	ARG	157	47.582	1.328	-8.084	1.00	0.00	3A4 3A4
ATOM	860		ARG	157	47.753	0.362	-7.136 -7.807	1.00	0.00	3A4
ATOM	861		ARG	157 157	47.975 42.316	2.607 1.305	-9.694	1.00	0.00	. 3A4
ATOM	862	0	ARG ARG	157	42.062		-10.749	1.00	0.00	3A4
ATOM ATOM	863 864	N	ASN	158	42.004	0.746	-8.509	1.00	0.00	3A4
ATOM	865	CA	ASN	158	41.363	-0.540	-8.359	1.00	0.00	3A4
ATOM	866	СВ	ASN	158	41.312	-0.962	-6.875	1.00	0.00	3A4
ATOM	867	CG	ASN	158	42.725	-1.184	-6.308	1.00	0.00	3A4
ATOM	868	OD1	ASN	158	43.710	-1.336	-7.029	1.00	0.00	3A4
ATOM	869	ND2	ASN	158	42.827	-1.211	-4.951	1.00	0.00	3A4
ATOM	870	С	ASN	15,8	39.959	-0.569	-8.928		0.00	3A4
MOTA	871	0	ASN	158	39.541	-1.568	-9.503	1.00	0.00	3A4 . 3A4
ATOM	872	N	LEU	159	39.205	0.547	-8.840 -9.460	1.00	0.00	3A4
ATOM	873	CA	LEU	159	37.900	0.698	-8.901	1.00	0.00	3A4
ATOM	874	CB	LEU	159	37.181	1.944	-7.590	1.00	0.00	3A4
ATOM	875	CG	LEU	159 159	36.392 35.846	1.845 3.252	-7.275	1.00	0.00	3A4
ATOM ATOM	876 877		LEU LEU	159	35.226	0.844	-7.672	1.00	0.00	3A4
ATOM	878	C	LEU	159	37.986		-10.979	1.00	0.00	3A4
ATOM	879	ŏ	LEU	159	37.180		-11.731	1.00	0.00	3A4
ATOM	880	N	ARG	160	39.032	1.542	-11.475	1.00	0.00	3A4
ATOM	881	CA	ARG	160	39.316		-12.887	1.00	0.00	3A4
ATOM	882	CB	ARG	160	40.462	2.697	-13.097	1.00	0.00	3A4
ATOM	883	CG	ARG	160	40.032		-12.829	1.00	0.00	3A4
MOTA	884	CD	ARG	160	41.097		-13.106		0.00	3A4 3A4
ATOM	885	NE	ARG	160	42.243		-12.147	1.00	0.00	3A4
ATOM	886	CZ	ARG	160	43.077		-11.785		0.00	3A4
ATOM	887		ARG	160	44.114 42.889		-10.932 -12.251		0.00	3A4
ATOM	888		ARG	160	39.687		-13.585		0.00	3A4
ATOM	889 890	C	ARG ARG	160 160	39.428		-14.767		0.00	3A4
ATOM ATOM	891	O N	ARG	161	40.250		-12.834		0.00	3A4
ATOM	892	CA	ARG	161	40.597		-13.293		0.00	3A4
ATOM	893	CB	ARG	161	41.743		-12.420		0.00	3A4
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ATOM	894	CG	ARG	161	43.082	-1.717 -12.670	1.00	0.00	3A4
ATOM	895	CD	ARG	161	44.093	-1.838 -11.519	1.00	0.00	3A4
MOTA	896	NE	ARG	161	44.400	-3.285 -11.257	1.00	0.00	3A4 3A4
ATOM	897	CZ NH1	ARG	161 161	45.172 45.396	-3.692 -10.198 -5.024 -10.010	1.00 1.00	0.00	3A4
ATOM	898 899	NH1		161	45.720	-2.792 -9.328	1.00	0.00	3A4
ATOM ATOM	900	C	ARG	161	39.432	-2.837 -13.270	1.00	0.00	3A4
ATOM	901	ŏ	ARG	161	39.618	-4.026 -13.474	1.00	0.00	3A4
ATOM	902	N	GLU	162	38.181	-2.341 -13.060	1.00	0.00	3A4
ATOM	903	CA	GLU	162	36.943	-3.106 -13.121	1.00 1.00	0.00	3A4 3A4
MOTA	904	CB	GLU GLU	162 162	35.704 35.006	-2.403 -12.447 -1.245 -13.229	1.00	0.00	3A4
ATOM ATOM	905 90 <b>6</b>	CG CD	GLU	162	33.961	-0.524 -12.375	1.00	0.00	3A4
ATOM	907		GLU	162	34.331	-0.002 -11.289	1.00	0.00	3A4
ATOM	908	OE2	GLU	162	32.779	-0.469 -12.809	1.00	0.00	3A4
ATOM	909	С	GLU	162	36.578	-3.419 -14.538	1.00	0.00	3A4 3A4
ATOM	910	0	GLU	162	36.521	-2.577 -15.435 -4.746 -14.788	1.00	0.00 0.00	3A4
ATOM	911 912	N CA	ALA ALA	163 163	36.386 36.408	-5.391 -16.091	1.00	0.00	3A4
MOTA MOTA	913	CB	ALA	163	37.029	-6.809 -15.993	1.00	0.00	3A4
ATOM	914	c	ALA	163	35.037	-5.494 -16.717	1.00	0.00	3A4
ATOM	915	0	ALA	163	34.019	-5.308 -16.051	1.00	0.00	3A4
ATOM	916	N	GLU	164	35.042	-5.771 -18.059	1.00 1.00	0.00 0.00	3A4 3A4
ATOM	917	CA	GLU	164 164	33.935 32.661	-5.860 -19.009 -6.587 -18.459	1.00	0.00	3A4
ATOM ATOM	918 919	CB CG	GLU	164	31.701	-7.151 -19.531	1.00	0.00	3A4
ATOM	920	CD	GLU	164	30.505	-7.813 -18.839	1.00	0.00	3A4
ATOM	921	OE1	GLÜ	164	29.737	-7.082 -18.156	1.00	0.00	3A4
ATOM	922		GLU	164	30.342	-9.055 -18.984	1.00	0.00 0.00	3A4 3A4
MOTA	923	C	GLU	164	33.612 32.462	-4.461 -19.520 -4.138 -19.797	1.00	0.00	3A4
ATOM ATOM	924 925	O N	GLU THR	164 165	34.671	-3.592 -19.572	1.00	0.00	3A4
ATOM	926	CA	THR	165	34.730	-2.131 -19.714	1.00	0.00	3A4
ATOM	927	СВ	THR	165	34.039	-1.480 -20.938	1.00	0.00	3A4
MOTA	928		THR	165	32.615	-1.557 -20.965	1.00	0.00	3A4 3A4
ATOM	929		THR	165	34.604 34.372	-2.115 -22.228 -1.470 -18.379	1.00	0.00	3A4
ATOM ATOM	930 931	С 0	THR THR	165 165	35.235	-0.931 -17.690	1.00	0.00	3A4
ATOM	932	N	GLY	166	33.075	-1.547 -17.996	1.00	0.00	3A4
ATOM	933	CA	GLY	166	32.567	-1.129 -16.720	1.00	0.00	3A4
MOTA	934	С	GLY	166		-1.094 -16.877		0.00	. 3A4 3A4
MOTA	935	0.	GLY	166	30.541 30.386	-0.151 -17.449 -2.143 -16.363		0.00	3A4
ATOM ATOM	936 937	N CA	LYS LYS	167 167	28.935	-2.211 -16.262		0.00	3A4
	. 938	CB	LYS	167		-3.202 -17.239		0.00	3A4
ATOM	939	CG	LYS	167	28.165	-2.770 -18.713		0.00	3A4
ATOM	940	CD	LYS	167	29.336	-3.252 -19.574		0.00 0.00	3A4 3A4
MOTA	941	CE	LYS	167	29.134 30.208	-2.949 -21.066 -3.554 -21.890		0.00	3A4
ATOM ATOM	942 943	NZ C	ĻYS LYS	167 167	28.582	-2.486 -14.802	1.00	0.00	3A4
ATOM	944	ō	LYS	167	27.816	-1.688 -14.271		0.00	3A4
ATOM	945	N	PRO	168	29.041	-3.521 -14.057		0.00	3A4
ATOM	946	CA	PRO	168	28.796	-3.641 -12.622		0.00	3A4 3A4
ATOM	947	CD	PRO	168 168	29.518 28.695	-4.787 -14.626 -5.165 -12.400		0.00	3A4
ATOM ATOM	948 949	CB CG	PRO PRO	168	29.625	-5.777 -13.459		0.00	3A4
ATOM	950	c	PRO	168	29.938	-3.027 -11.812	1.00	0.00	3A4
ATOM	951	0	PRO	168	31.100	-3.303 -12.110		0.00	3A4
ATOM	952	N	VAL	169	29.609	-2.275 <b>-</b> 10.724 -2.280 <b>-</b> 9.531		0.00	3A4 3A4
ATOM	953	CA	VAL VAL	169 169	30.441 31.674	-2.280 -9.531 -1.381 -9.591		0.00	3A4
ATOM ATOM	954 955	CB	VAL	169	31.356	0.130 -9.641			3A4
MOTA	956		VAL	169	32.702	-1.746 -8.502	1.00	0.00	3A4
MOTA	957	С	VAL	169	29.535	-1.926 -8.382			3A4
MOTA	958	0	VAL	169	28.623	-1.120 -8.520			3A4 3A4
MOTA	959	N	THR	170	29.805 29.193	-2.498 -7.184 -2.121 -5.93			3A4
MOTA	960 961	CA CB	THR THR	170 170	28.902	-3.314 -5.03			3A4
MOTA MOTA	962		THR	170	28.066	-4.231 -5.73	4 1.00	0.00	3A4
ATOM	963		THR	170	28.173	-2.877 -3.73			3A4
MOTA	964	C	THR	170	30.178	-1.183 -5.30 <sup>1</sup>			3A4 3A4
MOTA	965	0	THR	170	31.232	-1.589 -4.83	1 1.00	, 0.00	SAA

MOTA	966	N	LEU	171	29.854	0.126	-5.296	1.00	0.00	3A4
MOTA	967	CA	LEU	171	30.705	1.177	-4.769	1.00	0.00	3A4 3A4
ATOM	968	CB	LEU	171 171	30.055 30.547	2.555 3.319	-5.044 -6.282	1.00	0.00	3A4
MOTA MOTA	969 970	CG CD1	LEU	171	29.654	4.563	-6.453	1.00	0.00	3A4
ATOM	971	CD2		171	32.040	3.710	-6.194	1.00	0.00	3A4
ATOM	972	С	LEU	171	30.998	1.069	-3.277	1.00	0.00	3A4
MOTA	973	0	LEU	171	32.076	1.436	-2.831	1.00	0.00	3A4 3A4
ATOM	974	N CA	LY5	172 172	30.072 30.261	0.510 0.291	-2.464 -1.041	1.00	0.00	3A4
ATOM ATOM	975 976	CB	LYS	172	28.920	-0.132	-0.376	1.00	0.00	3A4
ATOM	977	CG	LYS	172	28.909	-0.334	1.158	1.00	0.00	3A4
ATOM	978	CD	LYS	172	29.194	0.939	1.969	1.00	0.00	3A4 3A4
ATOM	979	CE	LYS	172 172	29.078 30.110	0.766 -0.160	3.488 4.012	1.00	0.00	3A4
ATOM ATOM	980 981	NZ C	LYS	172	31.330	-0.744	-0.748	1.00	0.00	3A4
ATOM	982	ō	LYS	172	32.274	-0.492	-0.010	1.00	0.00	3A4
MOTA	983	N	ASP	173	31.243	-1.937	-1.374	1.00	0.00	3A4
MOTA	984	CA	ASP	173	32.134 31.447	-3.048 -4.365	-1.103 -1.539	1.00	0.00	3A4 3A4
ATOM ATOM	985 986	CB CG	ASP ASP	173 173	32.095	-5.634	-0.940	1.00	0.00	3A4
ATOM	987		ASP	173	32.129	-5.750	0.315	1.00	0.00	3A4
ATOM	988	OD2	ASP	173	32.559	-6.496	-1.735	1.00	0.00	3A4
MOTA	989	C	ASP	173	33.491	-2.909	-1.760	1.00	0.00	3A4 3A4
ATOM	990 991	O N	ASP VAL	173 174	34.487 33.571	-3.361 -2.272	-1.199 -2.947	1.00	0.00	· 3A4
ATOM ATOM	992	CA	VAL	174	34.804	-2.128	-3.702	1.00	0.00	3A4
ATOM	993	CB	VAL	174	34.550	-2.192	-5.209	1.00	0.00	3A4
MOTA	994		VAL	174	35.866	-2.225	-6.033	1.00	0.00 0.00	3A4 3A4
ATOM	995		VAL VAL	174 174	33.783 35.560	-3.513 -0.866	-5.482 -3.321	1.00	0.00	3A4
ATOM ATOM	996 997	c o	VAL	174	36.767	-0.793	-3.522	1.00	0.00	3A4
ATOM	998	N	PHE	175	34.889	0.162	-2.748	1.00	0.00	3A4
ATOM	999	CA	PHE	175	35.513	1.457	-2.585	1.00	0.00	3A4 3A4
ATOM	1000	CB	PHE	175 175	34.996 35.738	2.458 3.789	-3.637 -3.669	1.00	0.00	3A4
ATOM ATOM	1001 1002	CG CD1	PHE	175	35.169	4.936	-3.079	1.00	0.00	3A4
ATOM	1003		PHE	175	37.019	3.896	-4.239	1.00	0.00	3A4
ATOM	1004		PHE	175	35.866	6.153	-3.047	1.00	0.00	3A4 3A4
ATOM	1005		PHE	175 175	37.703 37.136	5.120 6.244	-4.237 -3.628	1.00	0.00	3A4
ATOM ATOM	1006 1007	CZ C	PHE	175	35.362	1.997	-1.219	1.00	0.00	3A4
ATOM	1008	ŏ	PHE	175	36.347	2.184	-0.509	1.00	0.00	3A4
ATOM	1009	N	GLY	176	34.105	2.318	-0.836	1.00	0.00	. 3A4 3A4
ATOM	1010	CA	GLY	176 176	33.755 34.098	3.060 2.332	0.352 1.609	1.00	0.00	3A4
ATOM ATOM	1011 1012	С 0	GLY GLY	176	34.413	2.958	2.614	1.00	0.00	3A4
ATOM	1013	N	ALA	177	34.126	0.976	1.565	1.00	0.00	3A4
ATOM	1014	CA	ALA	177	34.485	. 0.144	2.688	1.00	0.00	. 3A4
ATOM	1015	СВ	ALA	177	33.968 35.962	-1.294 0.124	2.532 2.957	1.00	0.00	3A4 3A4
ATOM ATOM	1016 1017	С 0	ALA ALA	177 177	36.406	0.124	4.080	1.00	0.00	3A4
ATOM	1018	N	TYR	178	36.777	-0.058	1.903	1.00	0.00	3A4
ATOM	1019	CA	TYR	178	38.203	-0.242	2.016		0.00	3A4
ATOM	1020	CB	TYR	178	38.721	-0.724 -2.235	0.638 0.593	1.00	0.00	3A4 3A4
MOTA MOTA	1021 1022	CG CD1	TYR TYR	178 178	38.656 37.893	-2.854	-0.416	1.00	0.00	3A4
ATOM	1023		TYR	178	39.236	-3.052	1.584	1.00	0.00	3A4
MOTA	1024		TYR	178	37.711	-4.243	-0.441	1.00	0.00	3A4
ATOM	1025		TYR	178	39.039 38.282	-4.442 -5.040	1.580 0.562	1.00	0.00	3A4 3A4
ATOM ATOM	1026 1027	CZ OH	TYR TYR	178 178	38.282	-6.439	0.553	1.00	0.00	3A4
ATOM	1028	c	TYR	178	38.966	1.017	2.362	1.00	0.00	3A4
ATOM	1029	0	TYR	178	39.918	0.985	3.127	1.00		3A4
MOTA	1030	N	SER	179	38.545	2.180 3.471	1.822 2.018	1.00		3A4 3A4
ATOM ATOM	1031 1032	CA CB	SER SER	179 179	39.171 38.412	4.545	1.196	1.00		3A4
ATOM	1032	OG	SER		39.108	5.787	1.074	1.00	0.00	3A4
MOTA	1034	С	SER	179	39.344	3.878	3.465	1.00		3A4
MOTA	1035	0	SER		40.445	4.039	3.966	1.00		3A4 3A4
ATOM ATOM	1036 1037	N CA	MET MET	180 180	38.263 38.328	3.919 4.314	4.233 5.621	1.00		3A4 3A4
MILLIM	103/	UM.	1.10.1	100	23.320	7.517	J. V.			

ATOM	1038	СВ	MET	180	36.898	4.623	5.984	1.00	0.00	3A4
MOTA	1039	CG	MET	180	36.729	5.941	5.189	1.00	0.00	3A4
ATOM	1040	SD	MET	180	35.589	5.903	3.791	1.00	0.00	3A4
ATOM	1041	CE	MET	180	36.564	7.153	2.893	1.00	0.00	3A4
ATOM	1042	C	MET	180	38.961	3.325	6.527	1.00	0.00	3A4 3A4
ATOM	1043	0	MET	180	39.602	3.684	7.513 6.144	1.00	0.00	3A4
ATOM	1044	N	ASP	181	38.892 39.455	2.030 1.016	6.971	1.00	0.00	3A4
ATOM	1045	CA	ASP ASP	181 181	38.927	-0.386	6.705	1.00	0.00	3A4
atom Atom	1046 1047	CB CG	ASP	181	38.781	-1.148	5.400	1.00	0.00	3A4
ATOM	1047		ASP	181	39.773	-1.165	4.635	1.00	0.00	3A4
ATOM	1049		ASP	181	37.728	-1.810	5.195	1.00	0.00	3A4
ATOM	1050	C	ASP	181	40.963	0.976	6.884	1.00	0.00	3A4
ATOM	1051	Ō	ASP	181	41.663	0.876	7.886	1.00	0.00	3A4
ATOM	1052	N	VAL	182	41.515	1.163	5.671	1.00	0.00	3A4
ATOM	1053	CA	VAL	182	42.946	1.238	5.464	1.00	0.00	3A4
MOTA	1054	CB	VAL	182	43.279	1.227	4.010	1.00	0.00	3A4
ATOM	1055		VAL	182	44.767	1.508	3.706	1.00	0.00	3A4
ATOM	1056		VAL	182	42.889	-0.181	3.532	1.00	0.00	3A4 3A4
ATOM	1057	C	VAL	182	43.593	2.408	6.151	1.00	0.00	3A4
ATOM	1058	0	VAL	182	44.676 42.877	2.298 3.540	6.708 6.210	1.00	0.00	3A4
MOTA MOTA	1059 1060	N CA	ILE	183 183	43.341	4.740	6.855	1.00	0.00	3A4
ATOM	1061	CB	ILE	183	42.480	5.913	6.432	1.00	0.00	3A4
ATOM	1062		ILE	183	42.783	7.205	7.220	1.00	0.00	3A4
ATOM	1063		ILE	183	42.712	6.215	4.926	1.00	0.00	3A4
ATOM	1064	CD	ILE	183	44.121	6.672	4.516	1.00	0.00	3A4
ATOM	1065	С	ILE	183	43.365	4.589	8.352	1.00	0.00	3A4
ATOM	1066	0	ILE	183	44.321	4.972	9.017	1.00	0.00	3A4
ATOM	1067	N	THR	184	42.323	3.969	8.947	1.00	0.00	3A4
ATOM	1068	CA	THR	184	42.311	3.780	10.379	1.00	0.00	3A4
ATOM	1069	СВ	THR	184	40.896	3.599	10.968	1.00	0.00	3A4 3A4
ATOM	1070		THR	184	40.842	3.873 2.222	12.369 10.686	1.00	0.00	3A4
ATOM	1071		THR	184 184	40.253 43.288	2.710	10.811	1.00	0.00	3A4
ATOM ATOM	1072 1073	С О	THR	184	43.934	2.838	11.842	1.00	0.00	3A4
ATOM	1074	N	SER	185	43.544	1.697	9.955	1.00	0.00	3A4
ATOM	1075	CA	SER	185	44.571	0.701	10.179	1.00	0.00	3A4
ATOM	1076	СВ	SER	185	44.486	-0.452	9.173	1.00	0.00	3A4
ATOM	1077	OG	SER	185	43.278	-1.178	9.354	1.00	0.00	3A4
ATOM	1078	C	SER	185	45.97 <b>5</b>	1.270	10.157	1.00	0.00	3A4
MOTA	1079		SER	185	46.793	0.962	11.011	1.00	0.00	3A4
MOTA	1080	N	THR	186	46.255	2.211	9.238	1.00	0.00	3A4
ATOM	1081	CA	THR	186	47.523	2.905	9.158	1.00	0.00	. 3A4 3A4
ATOM	1082	CB	THR	186	47.674	3.626 4.495	7.845 7.478	1.00	0.00	3A4
ATOM	1083		THR THR	186	46.613 47.869	2.559	6.746	1.00	0.00	3A4
ATOM ATOM	1084 1085	C	THR	186 186	47.770	3.895	10.256	1.00	0.00	3A4
ATOM	1086	Ö	THR	186	48.906	4.171	10.627	1.00	0.00	3A4
ATOM	1087	N	SER	187	46.676	4.433	10.825	1.00	0.00	3A4
ATOM	1088	CA	SER	187	46.674	5.311	11.961	1.00	0.00	3A4
ATOM	1089	СВ	SER	187	45.260	5.983	12.078	1.00	0.00	3A4
ATOM	1090	OG	SER	187	45.037	6.742	13.262	1.00	0.00	3A4
MOTA	1091	С	SER	187	47.012		13.221		0.00	3A4
MOTA	1092	0	SER	187	47.753	5.052	14.047	1.00	0.00	3A4 3A4
ATOM	1093	N	PHE	188	46.490	3.324	13.352	1.00	0.00	3A4
MOTA	1094	CA	PHE	188	46.634	2.477	14.511 14.609	1.00	0.00	3A4
ATOM	1095	CB	PHE	188 -188	45.408 44.440	1.520 2.221	15.507	1.00	0.00	3A4
ATOM ATOM	1096 1097	CG	PHE	188	43.828	3.428	15.112	1.00	0.00	3A4
ATOM	1098		PHE	188	44.425	1.853	16.860	1.00	0.00	3A4
ATOM	1099		PHE	188	43.309	4.298	16.068	1.00	0.00	3A4
MOTA	1100		PHE	188	43.917	2.727	17.815	1.00	0.00	3A4
ATOM	1101	CZ	PHE	188	43.370	3.945	17.418	1.00	0.00	3A4
MOTA	1102	С	PHE	188	47.882	1.665	14.537	1.00	0.00	3A4
MOTA	1103	0	PHE	188	48.386	1.332	15.605	1.00	0.00	3A4
ATOM	1104	N	GLY	189	48.414	1.335	13.350	1.00	0.00	3A4 3A4
ATOM	1105	CA	GLY	189	49.610	0.550	13.208	1.00	0.00	3A4
ATOM	1106	C	GLY	189	49.281 50.025	-0.923 -1.788	13.101 13.555	1.00		3A4
MOTA	1107	O N	GLY VAL	189 190	48.147	-1.240	12.428	1.00		3A4
MOTA MOTA	1108 1109	CA	VAL	190	47.745	-2.576	12.011	1.00		3A4
514 VII										

ATOM	1110	СВ	VAL	190	46.239	-2.768	11.929	1.00	0.00	3A4
ATOM	1111	CG1	VAL	190	45.823	-4.253	11.759	1.00	0.00	3A4
MOTA	1112	CG2		190	45.621	-2.217	13.235	1.00	0.00	3A4 3A4
MOTA	1113	C	VAL	190	48.306 48.419	-2.843 -1.948	10.635 9.801	1.00	0.00	3A4
ATOM	1114 1115	0 N	VAL ASN	190 191	48.419	-4.105	10.372	1.00	0.00	3A4
ATOM ATOM	1116	CA	ASN	191	49.636	-4.477	9.377	1.00	0.00	3A4
ATOM	1117	СВ	ASN	191	49.869	-5.997	9.517	1.00	0.00	3A4
ATOM	1118	CG	ASN	191	51.211	-6.502	8.934	1.00	0.00	3A4
ATOM	1119	OD1		191	52.277	-6.160	9.445	1.00	0.00	3A4 3A4
MOTA	1120	ND2		191	51.156	-7.322	7.848 7.970	1.00	0.00 0.00	3A4 3A4
ATOM	1121	C	ASN	191 191	49.394 48.268	-4.146 -4.363	7.523	1.00	0.00	3A4
ATOM ATOM	1122 1123	<b>и</b>	ASN ILE	192	50.505	-3.532	7.398	1.00	0.00	3A4
ATOM	1124	CA	ILE	192	50.796	-3.011	6.064	1.00	0.00	3A4
ATOM	1125	CB	ILE	192	49.572	-3.045	5.191	1.00	0.00	3A4
ATOM	1126	CG2		192	48.539	-2.012	5.843	1.00	0.00	3A4 3A4
ATOM	1127	CG1		192	49.850	-3.205	3.643 3.249	1.00	0.00	3A4
ATOM	1128	CD	ILE	192 192	50.855 51.332	-4.296 -1.562	6.101	1.00	0.00	3A4
ATOM ATOM	1129 1130	c o	ILE	192	51.714	-1.049	7.152	1.00	0.00	3A4
ATOM	1131	N	ASP	193	51.273	-0.876	4.912	1.00	0.00	3A4
ATOM	1132	CA	ASP	193	51.280	0.551	4.649	1.00	0.00	3A4
ATOM	1133	CB	ASP	193	52.500	0.950	3.755	1.00	0.00	3A4 3A4
MOTA	1134	CG	ASP	193	52.747	2.473	3.713	1.00	0.00 0.00	3A4
ATOM	1135		ASP	193	52.690 52.993	3.055 3.065	2.596 4.798	1.00	0.00	3A4
ATOM	1136 1137	C C	ASP ASP	193 193	49.942	0.941	3.982	1.00	0.00	3A4
ATOM ATOM	1138	ŏ	ASP	193	49.555	2.107	4.042	1.00	0.00	3A4
ATOM	1139	N	SER	194	49.199	-0.025	3.351	1.00	0.00	3A4
MOTA	1140	CA	SER	194	47.801	0.108	2.935	1.00	0.00	3A4 3A4
MOTA	1141	CB	SER	194	47.674	0.859	1.564	1.00	0.00	3A4
ATOM	1142	OG	SER	194 194	48.568 47.072	0.364 -1.263	0.570 2.877	1.00	0.00	3A4
ATOM .	1143 1144	C O	SER SER	194	47.201	-1.949	1.864	1.00	0.00	3A4
ATOM	1145	N	LEU	195	46.300	-1.682	3.968	1.00	0.00	3A4
ATOM	1146	CA	LEU	195	45.506	-2.928	4.205	1.00	0.00	3A4
MOTA	1147	CB	LEU	195	44.616	-3.155	2.908	1.00	0.00	3A4 3A4
MOTA	1148	CG	LEU	195	43.358	-4.046	2.893 1.614	1.00	0.00	3A4
MOTA	1149		LEU	195 195	42.566 43.591	-3.731 -5.569	2.963	1.00	0.00	3A4
ATOM ATOM	1150 1151	CDZ	LEU LEU	195	46.313	-4.231	4.384	1.00	0.00	3A4
ATOM	1152	ŏ	LEU	195	46.823	-4.525	3.303	1.00	0.00	3A4
ATOM	1153	N	ASN	196	46.462	-5.133	5.522	1.00	0.00	3A4
MOTA	1154	CA	ASN	196	46.660	-6.447	5.007	1.00	0.00	3A4 3A4
MOTA	1155	CB	ASN	196	48.141	-6.561	4.645 3.641	1.00	0.00	3A4
ATOM	1156	CG.	ASN	196 196	48.532 49.287	-7.677 -8.581	3.992	1.00	0.00	3A4
ATOM ATOM	1157 1158		ASN ASN	196	48.039	-7.601	2.374		0.00	3A4
ATOM	1159	C	ASN	196	46.000	-7.578	5.603	1.00	0.00	3A4
ATOM	1160	Ó	ASN	196	44.826	-7.879	5.338	1.00	0.00	3A4
MOTA	1161	N	ASN	197	46.757	-8.297	6.407		0.00	3A4 3A4
MOTA	1162	CA	ASN	197	46.317	-9.599	6.859 7.443	1.00	0.00	3A4
MOTA	1163 1164	CB CG	ASN ASN	197 197		-10.511 -10.689	6.405	1.00	0.00	3A4
ATOM ATOM	1165		ASN	197		-11.249	5.336	1.00	0.00	3A4
ATOM	1166		ASN	197		-10.219	6.717	1.00	0.00	3A4
ATOM	1167	¢	ASN	197	45.160	-9.556	7.804	1.00	0.00	3A4
MOTA	1168	0	ASN	197		-10.439	7.761	1.00	0.00	3A4 3A4
MOTA	1169	N	PRO	198	45.075 44.013	-8.496 -8.420	8.595 9.555	1.00	0.00	3A4
MOTA MOTA	1170 1171	CA CD	PRO PRO	198 198	44.013	-7.818	9.154	1.00		3A4
ATOM	1171	CB	PRO	198	44.652	-7.631	10.641	1.00		3A4
ATOM	1173	CG	PRO	198	46.123	-7.908	10.628	1.00		3A4
ATOM	1174	С	PRO	198	42.754	-7.786	9.085	1.00		3A4
MOTA	1175	0	PRO	198	41.799	-7.743	9.865	1.00		3A4 3A4
MOTA	1176	N	GLN	199	42.701 41.636	-7.279 -6.407	7.830 7.407	1.00		3A4
ATOM ATOM	1177 1178	CA CB	GLN GLN	199 199	41.636	-5.668	6.066	1.00		3A4
ATOM	1178	CG	GLN	199	41.001	-4.419	5.844	1.00		3A4
MOTA	1180	CD	GLN		41.471	-3.266	6.742	1.00	0.00	3A4
ATOM	1181		GLN		42.353	-2.503	6.348	1.00	0.00	3A4

ATOM	1182	NE2	GLN	199	40.885	-3.125	7.963	1.00	0.00	3A4
ATOM	1183	С	GLN	199	40.319	-7.071	7.338	1.00	0.00	3A4
MOTA	1184	0	GLN	199	39.374	-6.533	7.889 6.717	1.00	0.00	3A4 3A4
ATOM	1185	N	ASP ASP	200 200	40.193 38.939	-8.262 -8.983	6.597	1.00	0.00	3A4
MOTA MOTA	1186 1187	CA CB	ASP	200	39.049 -		5.538	1.00	0.00	3A4
ATOM	1188	CG	ASP	200	37.683 -		5.079	1.00	0.00	3A4
MOTA	1189	OD1		200	37.459 -		5.238	1.00	0.00	3A4 3A4
MOTA	1190	OD2		200	36.855 38.347	-9.893 -9.432	4.566 7.927	1.00	0.00	3A4
MOTA MOTA	1191 1192	С 0	ASP ASP	200 200	37.137	-9.315	8.099	1.00	0.00	3A4
ATOM	1193	N	PRO	201	39.155	-9.847	8.917	1.00	0.00	3A4
ATOM	1194	CA	PRO	201	38.699		10.270	1.00	0.00	3A4 3A4
MOTA	1195	CD	PRO	201	40.343 · 39.936 ·		8.654 11.012	1.00	0.00	3A4
ATOM ATOM	1196 1197	CB CG	PRO PRO	201 201	40.633		9.938	1.00	0.00	3A4
ATOM	1198	c	PRO	201	38.128	-8.916	10.997	1.00	0.00	3A4
ATOM	1199	0	PRO	201	37.076	-9.052	11.615	1.00	0.00 0.00	3A4 3A4
ATOM	1200	N	PHE	202	38.762	-7.733 -6.521	10.872 11.530	1.00	0.00	3A4
ATOM	1201	CA CB	PHE PHE	202 202	38.319 39.462	-5.473	11.494	1.00	0.00	3A4
ATOM ATOM	1202 1203	CG	PHE	202	40.009	-5.259	12.888	1.00	0.00	3A4
ATOM	1204		PHE	202	40.365	-6.366	13.691	1.00	0.00	3A4 3A4
ATOM	1205		PHE	202	40.293	-3.968	13.372 14.987	1.00	0.00 0.00	3A4
MOTA	1206		PHE PHE	202 202	40.856 40.855	-6.184 -3.790	14.647	1.00	0.00	3A4
ATOM ATOM	1207 1208	CZ	PHE	202	41.107	-4.894	15.465	1.00	0.00	3A4
ATOM	1209	C	PHE	202	37.080	-5.964	10.887	1.00	0.00	3A4 3A4
MOTA	1210	0	PHE	202	36.208	-5.444	11.573 9.554	1.00	0.00	3A4 3A4
MOTA	1211	N CA	VAL VAL	203 203	36.928 35.752	-6.145 -5.762	8.799	1.00	0.00	3A4
ATOM ATOM	1212 1213	CB	VAL	203	36.015	-5.808	7.287	1.00	0.00	3A4
ATOM	1214		VAL	203	34.738	-5.677	6.411	1.00	0.00	3A4 3A4
ATOM	1215		VAL	203	36.983	-4.648	6.954 9.199	1.00	0.00	3A4
MOTA	1216	C	VAL VAL	203 203	34.545 33.451	-6.596 -6.068	9.155	1.00	0.00	3A4
ATOM ATOM	1217 1218	O N	GLU	204	34.736	-7.908	9.475	1.00	0.00	3A4
ATOM	1219	CA	GLU	204	33.684	-8.782	9.967	1.00	0.00	3A4
ATOM	1220	СВ	GLU	204		-10.262	9.912 8.472	1.00	0.00	3A4 3A4
ATOM	1221	CG CD	GLU	204 204		-10.797 -12.210	8.489	1.00	0.00	3A4
ATOM ATOM	1222 1223		GLU	204		-12.394	7.934	1.00	0.00	3A4
ATOM	1224		GLU	204		-13.123	9.059	1.00	0.00	3A4 3A4
MOTA	1225	C	GLU	204	33.230	-8.440	11.373	1.00	0.00	3A4
MOTA	1226	<b>И</b>	GLU ASN	204 205	32.042 34.176	-8.449 -8.057	12.259	1.00	0.00	3A4
ATOM ATOM	1227 1228	CA	ASN	205	33.914	-7.660	13.628	1.00	0.00	. 3A4
MOTA	1229	CB	ASN	205	35.248	-7.438	14.383	1.00	0.00 0.00	3A4 3A4
MOTA	1230	CG	ASN	205	36.015	-8.751 -8.776	14.628	1.00	0.00	3A4
ATOM	1231 1232		ASN ASN	205 205	37.233 35.329	-9.842	15.069	1.00	0.00	3A4
MOTA MOTA	1233	C	ASN	205	33.087	-6.395	13.736	1.00	0.00	3A4
ATOM	1234	0	ASN	205	32.115	-6.344	14.487	1.00	0.00	3A4 3A4
ATOM	1235	N	THR	206	33.414 32.762	-5.376 -4.077	12.903 12.899	1.00	0.00 0.00	3A4
ATOM	1236 1237	CA CB	THR THR	206 206	33.525	-3.007	12.102	1.00		3A4
MOTA MOTA	1238		THR	206	34.406	-3.549	11.139	1.00		3A4
ATOM	1239	CG2	. THR	206	34.381	-2.246	13.141	1.00		3A4 3A4
MOTA	1240	C	THR	206	31.364 30.435	-4.178 -3.581	12.322 12.843	1.00		3A4
ATOM ATOM	1241 1242	O N	THR LYS	206 207	31.178	-5.009	11.279	1.00		3A4
ATOM	1243	CA	LYS	207	29.905	-5.266	10.645	1.00		3A4
MOTA	1244	СВ	LYS	207	30.122	-6.061	9.349	1.00		3A4 3A4
ATOM	1245	CG	LYS	207	28.927 29.306	-6.211 -6.802	8.393 7.027			3A4
MOTA MOTA	1246 1247	CE	LYS LYS	207 207	29.832	-8.246	7.088		0.00	3A4
MOTA	1248	NZ	LYS	207	30.150	-8.750	5.731	1.00		3A4
ATOM	1249	C	LYS	207	28.938		11.523			3A4 3A4
MOTA	1250		LYS	207	27.753 29.441	-5.736 -6.958	11.533 12.359			3A4
ATOM	1251 1252		LYS LYS		28.646					3A4
ATOM ATOM	1252				29.443					3A4

АТОМ	1254	CG	LYS	208	28.627	-9.993	14.610	1.00	0.00		3A4
ATOM	1255	CD	LYS	208	29.414		15.031	1.00	0.00		3A4 3A4
ATOM	1256	CE	LYS	208	29.894 - 31.125 -	-12.177	13.900 13.236	1.00	0.00		3A4
ATOM	1257 1258	NZ C	LYS LYS	208 208	28.094	-6.905	14.430	1.00	0.00		3A4
ATOM ATOM	1259	ŏ	LYS	208	26.931	-7.047	14.780	1.00	0.00		3A4
ATOM	1260	N	LEU	209	28.886	-5.983	15.022	1.00	0.00		3A4
MOTA	1261	CA	LEU	209	28.454	-5.149	16.133 16.784	1.00	0.00		3A4 3A4
ATOM	1262	CB CG	LEU	209 209	29.656 29.353	-4.415 -3.397	17.945	1.00	0.00		3A4
ATOM ATOM	1263 1264	CD1		209	28.592	-4.009	19.146	1.00	0.00		3A4
ATOM	1265	CD2		209	30.596	-2.606	18.399	1.00	0.00		3A4
MOTA	1266	С	LEU	209	27.416	-4.112	15.737 16.507	1.00 1.00	0.00		3A4 3A4
ATOM	1267	О И	LEU	209 210	26.515 27.527	-3.793 -3.561	14.510	1.00	0.00		3A4
ATOM ATOM	1268 1269	CA	LEU	210	26.707	-2.449	14.080	1.00	0.00		3A4
ATOM	1270	СВ	LEU	210	27.559	-1.343	13.418	1.00	0.00		3A4
ATOM	1271	CG	LEU	210	28.684	-0.850	14.384	1.00	0.00		3A4 3A4
MOTA	1272		LEU	210 210	29.655 28.176	0.113 -0.257	13.699 15.717	1.00	0.00		3A4
ATOM ATOM	1273 1274	CDZ	LEU	210	25.611	-2.862	13.145	1.00	0.00		3A4
ATOM	1275	ŏ	LEU	210	24.465	-2.454	13.335	1.00	0.00		3A4
ATOM	1276	N	ARG	211	25.948	-3.571	12.035	1.00	0.00		3A4 3A4
ATOM	1277	CA	ARG	211	25.146 26.033	-3.650 -3.592	10.816 9.539	1.00	0.00		3A4
ATOM ATOM	1278 1279	CB CG	ARG ARG	211 211	26.927	-2.337	9.503	1.00	0.00		3A4
ATOM	1280	CD	ARG	211	27.841	-2.220	8.274	1.00	0.00		3A4
ATOM	1281	NE	ARG	211	27.005	-2.107	7.024	1.00	0.00 0.00		3A4 3A4
ATOM	1282	CZ	ARG	211 211	26.814 26.014	-0.939 -0.951	6.329 5.223	1.00	0.00		3A4
ATOM ATOM	1283 1284	NH1 NH2	ARG ARG	211	27.397	0.236	6.711	1.00	0.00		3A4
ATOM	1285	С	ARG	211	24.236	-4.864	10.757	1.00	0.00		3A4
MOTA	1286	0	ARG	211	23.275	-4.868	9.989	1.00	0.00		3A4 3A4
MOTA	1287	N	PHE	212 212	24.496 23.555	-5.910 -6.992	11.589 11.826	1.00	0.00		3A4
ATOM ATOM	1288 1289	CA CB	PHE	212	23.730	-8.273	10.930	1.00	0.00		3A4
ATOM	1290	CG	PHE	212	25.061	-8.998	10.978	1.00	0.00		3A4
ATOM	1291		PHE	212		-10.224	11.667	1.00	0.00		3A4 3A4
ATOM	1292	CD2		212 212	26.182 26.367	-8.527 -10.954	10.268 11.660	1.00 1.00	0.00		3A4
ATOM ATOM	1293 1294		PHE	212	27.380	-9.259	10.254	1.00	0.00		3A4
ATOM	1295	CZ	PHE	212		-10.469	10.952	1.00	0.00		3A4
MOTA	1296	C.		212	23.608	-7.246	13.314	1.00	0.00		3A4 3A4
ATOM	1297 1298	O N	PHE ASP	212 213	24.292 22.863	-8.143 -6.398	13.802 14.068		0.00		3A4
ATOM ATOM	1299	CA	ASP	213	22.843	-6.356	15.513	1.00	0.00		3A4
MOTA	1300	CB	ASP	213	23.642	-5.131	16.046	1.00	0.00		3A4 3A4
MOTA	1301	CG	ASP	213	23.916	-5.215	17.558 17.982	1.00	0.00		3A4
MOTA MOTA	1302 1303		ASP ASP	213 213	24.608 23.444	-6.179 -4.312	18.300	1.00	0.00	•	3A4
ATOM	1303	C	ASP	213	21.391	-6.281	15.902	1.00	0.00		3A4
ATOM	1305	0	ASP	213	20.714	-5.286	15.648	1.00	0.00		3A4 3A4
MOTA	1306	N	PHE	214	20.894 19.516	-7.371 -7.516	16.533 16.941	1.00	0.00		3A4
ATOM ATOM	1307 1308	CA CB	PHE	214 214	18.526	-7.900	15.776	1.00	0.00		3A4
ATOM	1309	CG	PHE	214	19.127	-8.826	14.734	1.00	0.00		3A4
ATOM	1310		PHE	214	19.610	-8.306	13.515	1.00	0.00		3A4 3A4
MOTA	1311		PHE	214 214	19.216 20.186	-10.215 -9.143	14.950 12.550	1.00	0.00		3A4
ATOM ATOM	1312 1313		PHE	214		-11.058	13.987	1.00	0.00		3A4
ATOM	. 1314	cz	PHE	214		-10.520	12.788	1.00	0.00		3A4
ATOM	1315	С	PHE	214	19.513	-8.554	18.034	1.00	0.00		3A4 3A4
ATOM	1316	0 N	PHE	214 215	20.344 18.527	-9.460 -8.428	18.058 18.956		0.00		3A4
ATOM ATOM	1317 1318	N CA	LEU	215	18.216	-9.384	19.995		0.00		3A4
MOTA	1319	СВ	LEU	215	18.914	-9.072	21.353		0.00		3A4
ATOM	1320	CG	LEU	215		-10.089	22.505		0.00		3A4 3A4
ATOM	1321		LEU LEU	215 215	19.075 19.419	-11.533 -9.639	22.128 23.783				3A4
MOTA MOTA	1322 1323	CDZ	LEU		16.716		20.078		0.00		3A4
ATOM	1324	ŏ	LEU	215	16.151	-8.667	20.970	1.00			3A4
ATOM	1325	N	ASP		16.046	-9.926	19.073	1.00	0.00		3A4

ATOM	1326	CA	ASP	216	14.627	-9.830	18.781	1.00	0.00	3A4
	1327	СВ	ASP	216		-9.623	17.242	1.00	0.00	3A4
ATOM			ASP	216	14.915 -		16.328	1.00	0.00	. 3A4
ATOM	1328	CG					16.241	1.00	0.00	3A4
ATOM	1329	ODI		216	16.161 -			1.00	0.00	3A4
ATOM	1330	OD2	ASP	216	14.075 -		15.700			
ATOM	1331	С	ASP	216	13.914 -	11.069	19.316	1.00	0.00	3A4
ATOM	1332	0	ASP	216	14.578 -	12.088	19.506	1.00	0.00	3A4
ATOM	1333	N	PRO	217	12.576 -	11.062	19.553	1.00	0.00	3A4
	1334	CA	PRO	217	11.794 -		19.974	1.00	0.00	3A4
ATOM						-9.819	19.695	1.00	0.00	3A4
ATOM	1335	CD	PRO	217				1.00	0.00	3A4
ATOM	1336	СВ	PRO	217	10.525 -		20.611			
ATOM	1337	CG	PRO	217	10.367 -		19.970	1.00	0.00	3A4
ATOM	1338	С	PRO	217	11.504 -	-13.148	18.786	1.00	0.00	3A4
ATOM	1339	0	PRO	217	12.309 -	-14.043	18.527	1.00	0.00	3A4
ATOM	1340	N	PHE	218	10.374 -	12.933	18.064	1.00	0.00	3A4
		CA	PHE	218	10.004 -		16.839	1.00	0.00	3A4
MOTA	1341				8.877 -		17.032	1.00	0.00	3A4
MOTA	1342	СВ	PHE	218				1.00	0.00	3A4
atom	1343	CG	PHE	218	9.294 -		18.036			
ATOM	1344	CD1	PHE	218	8.630 -		19.273	1.00	0.00	3A4
ATOM	1345	CD2	PHE	218	10.354 -	-16.621	17.766	1.00	0.00	3A4
ATOM	1346	CEL	PHE	218	9.018 -	-16.783	20.225	1.00	0.00	3A4
ATOM	1347		PHE	218	10.751 -	-17.572	18.720	1.00	0.00	3A4
				218	10.083 -		19.950	1.00	0.00	3A4
ATOM	1348	CZ	PHE				15.883	1.00	0.00	3A4
ATOM	1349	С	PHE	218	9.495 -					3A4
MOTA	1350	0	PHE	218		-12.860	14.737	1.00	0.00	
MOTA	1351	N	PHE	219	9.400 -	-11.297	16.374	1.00	0.00	3A4
MOTA	1352	CA	PHE	219	8.762 -	-10.165	15.736	1.00	0.00	3A4
ATOM	1353	СВ	PHE	219	7.558	-9.630	16.572	1.00	0.00	3A4
	1354	ĊĢ	PHE	219	6.443 -	-10.646	16.570	1.00	0.00	3A4
ATOM						-10.600	15.587	1.00	0.00	3A4
MOTA	1355		PHE	219			17.542	1.00	0.00	3A4
MOTA	1356		PHE	219		-11.664				3A4
ATOM	1357		PHE	219		-11.546	15.576	1.00	0.00	
ATOM	1358	CE2	PHE	219		-12.611	17.536	1.00	0.00	3A4
ATOM	1359	CZ	PHE	. 219	4.360 -	-12.551	16.553	1.00	0.00	3A4
ATOM	1360	С	PHE	219	9.798	-9.078	15.602	1.00	0.00	3A4
	1361	ō	PHE	219	10.805	~9.068	16.307	1.00	0.00	3A4
ATOM				220	9.547	-8.131	14.664	1.00	0.00	3A4
MOTA	1362	N	LEU			-7.050	14.321	1.00	0.00	3A4
ATOM	1363	CA	LEU	220	10.447				0.00	3A4
ATOM	1364	CB	LEU	220	11.550	-7.452	13.279	1.00		3A4
MOTA	1365	CG	LEU	220	11.130	-7.889	11.840	1.00	0.00	
ATOM	1366	CD1	LEU	220	12.368	-7.938		1.00	0.00	3A4
MOTA	1367	CD2	LEU	220	10.365	-9.229	11.764	1.00	0.00	3A4
ATOM	1368	c	LEU	220	9.590	-5.908	13.825	1.00	0.00	3A4
-				220	8.366	-5.964	13.937	1.00	0.00	3A4
MOTA	1369	0	LEU			-4.849	13.284	1.00	0.00	3A4
MOTA	1370	N	SER	221	10.268			1.00	0.00	3A4
MOTA	1371	CA	SER	221	9.781	-3.584	12.735			3A4
MOTA	1372	CB	SER	221	8.270	-3.542	12.288	1.00	0.00	
MOTA	1373	OG	SER	221	7,980	-2.485	11.376	1.00	0.00	3A4
ATOM	1374	С	SER	221	10.129	-2.514	13.764	1.00	<b>0.00</b>	3A4
ATOM	1375	ō	SER	221	10.958	-2.740	14.646	1.00	0.00	3A4
	1376	N	ILE	222	9.495	-1.312	13.661	1.00	0.00	3A4
ATOM					9.692	-0.155	14.524	1.00	0.00	3A4
MOTA	1377	CA	ILE	222			13.735	1.00	0.00	3A4
ATOM	1378	СВ	ILE	222	9.886	1.145			0.00	3A4
ATOM	1379	CG2	ILE	222	11.258	1.038	13.025	1.00		
ATOM	1380	CG1	ILE	222	8.727	1.449	12.741	1.00	0.00	3A4
ATOM	1381	CD	ILE	222	8.868	2.791	12.016	1.00	0.00	3A4
ATOM	1382	С	ILE	222	8.533	-0.038	15.500	1.00	0.00	3A4
ATOM	1383	ŏ	ILE	222	8.631	0.670	16.501	1.00	0.00	3A4
				223	7.406	-0.746	15.215	1.00	0.00	3A4
MOTA	1384	N	THR				16.050	1.00	0.00	3A4
ATOM	1385	CA	THR	223	6.225	-0.787			0.00	3A4
ATOM	1386	СВ	THR	223	5.259	0.384	15.782	1.00		3A4
MOTA	1387	OG1	THR	223	4.159	0.414	16.691	1.00	0.00	
ATOM	1388	CG2	THR	223	4.751	0.459	14.318	1.00	0.00	3A4
ATOM	1389	c	THR	223	5.633	-2.165	15.811	1.00	0.00	3A4
ATOM	1390	ŏ	THR	223	5.360	-2.558	14.678	1.00	0.00	3A4
			VAL	224	5.435	-2.927	16.918	1.00	0.00	3A4
ATOM	1391	N			4.832	-4.244	16.917	1.00	0.00	3A4
MOTA	1392	CA	VAL	224				1.00	0.00	3A4
MOTA	1393	CB	VAL	224	5.751	-5.354	16.379			3A4
MOTA	1394	CG1	VAL	224	7.065	-5.517	17.186		0.00	
ATOM	1395	CG2	VAL	224	4.973	-6.679	16.198		0.00	3A4
ATOM	1396	c	VAL	224	4.397	-4.468	18.349	1.00	0.00	3A4
MOTA	1397	ŏ	VAL	224	5.085	-4.071	19.290		0.00	3A4
ATOM	1331	9	• ^ ~							

ATOM	1398	N	PHE	225	3.212 -5.114	18.534	1.00	0.00		3A4
ATOM	1399	CA	PHE	225	2.568 -5.398	19.809	1.00	0.00		3A4
ATOM	1400	СВ	PHE	225	1.025 -5.112	19.736	1.00	0.00		3A4
ATOM	1401	CG	PHE	225	0.345 -5.089	21.089	1.00	0.00		3A4
MOTA	1402	CD1		225	0.584 -4.036	21.993	1.00	0.00		3A4
MOTA	1403	CD2		225	-0.533 -6.123	21.470	1.00	0.00		3A4 3A4
MOTA	1404	CEl		225	-0.038 -4.017	23.251	1.00	0.00		3A4
ATOM	1405	CE2		225	-1.156 -6.107	22.726 23.617	1.00	0.00		3A4
MOTA	1406	cz	PHE	225	-0.908 -5.053 2.898 -6.812	20.313	1.00	0.00		3A4
ATOM	1407	C	PHE	225 225	3.306 -6.885	21.472	1.00	0.00		3A4
ATOM	1408	O N	PHE PRO	226	2.776 -7.964	19.590	1.00	0.00		3A4
MOTA MOTA	1409 1410	CA	PRO	226	3.087 -9.298	20.117	1.00	0.00		3A4
ATOM	1411	CD	PRO	226	2.027 -8.062	18.335	1.00	0.00		3A4
ATOM	1412	СВ	PRO	226	2.324 -10.268	19.186	1.00	0.00		3A4
ATOM	1413	CG	PRO	226	2.191 -9.507	17.865	1.00	0.00		3A4
ATOM	1414	С	PRO	226	4.587 -9.598	20.127	1.00	0.00		3A4
ATOM	1415	0	PRO	226	5.346 -9.003	19.361	1.00	0.00		3A4
ATOM	1416	N	PHE	227	4.993 -10.544	21.009	1.00	0.00		3A4 3A4
ATOM	1417	CA	PHE	227	6.356 -10.995	21.212	1.00	0.00		3A4
MOTA	1418	СВ	PHE	227	7.106 -10.254	22.376	1.00	0.00 0.00		3A4
MOTA		CG	PHE	227	6.298 -10.129 5.437 -9.031	23.651 23.855	1.00	0.00		3A4
MOTA	1420		PHE	227	5.437 -9.031 6.393 -11.105	24.663	1.00	0.00		3A4
ATOM	1421		PHE	227	4.677 -8.920	25.028	1.00	0.00		3A4
ATOM	1422		PHE	227 227	5.634 -10.999	25.838	1.00	0.00		3A4
MOTA MOTA	1423 1424	CZ	PHE	227	4.775 -9.907	26.019	1.00	0.00		3A4
ATOM	1425	c	PHE	227	6.307 -12.495	21.429	1.00	0.00		3A4
ATOM	1426	ō	PHE	227	7.291 -13.188	21.177	1.00	0.00		3A4
ATOM	1427	N	LEU	228	5.134 -13.001	21.925	1.00	0.00		3A4
ATOM	1428	CA	LEU	228	4.753 -14.389	22.186	1.00	0.00		3A4
ATOM.	1429	СВ	LEU	228	5.137 -15.381	21.024	1.00	0.00		3A4
MOTA	1430	CG	LEU	228	4.217 -16.607	20.757	1.00	0.00		3A4
ATOM	1431		LEU	228	4.267 -17.707	21.832	1.00	0.00		3A4 3A4
ATOM	1432		LEU	228	2.767 -16.215	20.406	1.00	0.00		3A4
ATOM	1433	C	LEU	228	5.274 -14.788	23.565 24.575	1.00	0.00		3A4
ATOM	1434	0	LEU	228	4.778 -14.291 6.316 -15.659	23.623	1.00	0.00		3A4
MOTA	1435	N	ILE	229 229	7.097 -15.948	24.811	1.00	0.00		3A4
ATOM	1436 1437	CA CB	ILE	229	6.457 -16.944	25.799	1.00	0.00		3A4
ATOM ATOM	1438		ILE	229	6.056 -18.311	25.188	1.00	0.00		3A4
ATOM	1439		ILE	229	7.185 -17.043	27.173	1.00	0.00		3A4
ATOM	1440	CD	ILE	229	8.372 -18.014	27.278	1.00	0.00		3A4
ATOM	1441	С	ILE	229	8.458 -16.351	24.252	1.00	0.00		3A4
ATOM	1442	0	ILE	229	8.631 -17.503	23.857	1.00	0.00		3A4
ATOM	1443	N	PRO	230	9.474 -15.455	24.157	1.00	0.00	; ,	3A4 3A4
ATOM	1444	CA	PRO	230	10.759 -15.735	23.519	1.00	0.00 0.00		3A4
MOTA	1445	CD	PRO	230	9.306 -14.022	24.410	1.00	0.00		3A4
MOTA	1446	СВ	PRO	230	11.244 -14.349 10.655 -13.376	23.055	1.00	0.00		3A4
ATOM	1447	CG	PRO	230 230	11.749 -16.380	24.483	1.00	0.00		3A4
ATOM ATOM	1448 1449	C O	PRO	230	11.509 -16.422	25.691	1.00	0.00		3A4
ATOM	1450	N	ILE	231	12.894 -16.870	23.931	1.00	0.00		3A4
ATOM	1451	CA	ILE	231	13.997 -17.495	24.644	1.00	0.00		3A4
ATOM	1452	СВ	ILE	231	14.463 -18.802	23.988	1.00	0.00		3A4
ATOM	1453		ILE	231	15.554 -19.489	24.852	1.00	0.00		3A4
ATOM	1454	CG1	ILE	231	13.275 -19.767	23.714	1.00	0.00		3A4
ATOM	1455	CD	ILE	231	12.502 -20.240	24.953	1.00	0.00		3A4
ATOM	1456	С	ILE	231	15.116 -16.473	24.709	1.00	0.00		3A4 3A4
ATOM	1457	0	ILE	231	15.691 -16.247	25.773	1.00	0.00 0.00		3A4
MOTA	1458	N	LEU	232	15.428 -15.844	23.533	1.00	0.00		3A4
ATON	1459	CA	LEU	232	16.397 -14.778 16.312 -13.552	23.277 24.250	1.00	0.00		3A4
MOTA	1460	CB	LEU	232 232	14.944 -12.824	24.269	1.00	0.00		3A4
ATOM	1461 1462	CG CD1	LEU	232	14.900 -11.763	25.383	1.00	0.00		3A4
MOTA MOTA	1462		LEU	232	14.567 -12.203	22.908	1.00	0.00		3A4
ATOM	1464	C	LEU	232	17.814 -15.328	23.232	1.00	0.00		3A4
MOTA	1465	ŏ	LEU	232	18.606 -15.133	24.154	1.00	0.00		3A4
ATOM	1466	N	GLU	233	18.131 -16.047	22.125	1.00	0.00		3A4
MOTA	1467	CA	GLU	233	19.390 -16.728	21.896				3A4
ATOM	1468	СВ	GLU	233	19.269 -18.268	22.115				3A4
MOTA	1469	CG	GLU	233	18.095 -18.955	21.373	1.00	0.00		3A4

ATOM	1470	CD	GLU	233	18.120 -20.462 21.648 1.00 0.00	3A4
ATOM	1471	OE1	GLU	233	19.140 -21.114 21.295 1.00 0.00	3A4 3A4
ATOM	1472	OE2		233	17.118 -20.985 22.205 1.00 0.00 19.828 -16.395 20.489 1.00 0.00	3A4
ATOM	1473	C O	GLU GLU	233 233	19.828 -16.395 20.489 1.00 0.00 20.256 -17.261 19.726 1.00 0.00	3A4
ATOM ATOM	1474 1475	N	VAL	234	19.734 -15.088 20.125 1.00 0.00	3A4
ATOM	1476	CA	VAL	234	20.053 -14.558 18.815 1.00 0.00	3A4
MOTA	1477	СВ	VAL	234	18.792 -14.275 17.987 1.00 0.00 17.739 -13.402 18.723 1.00 0.00	3A4 3A4
ATOM	1478	CG1		234	17.739 -13.402 18.723 1.00 0.00 19.142 -13.768 16.568 1.00 0.00	3A4
ATOM ATOM	1479 1480	CG2 C	VAL	234 234	20.960 -13.370 19.064 1.00 0.00	3A4
ATOM	1481	ŏ	VAL	234	20.563 -12.209 18.984 1.00 0.00	3A4
ATOM	1482	N	LEU	235	22.242 -13.673 19.393 1.00 0.00	3A4 3A4
MOTA	1483	CA	LEU	235	23.270 -12.694	3A4
MOTA	1484 1485	CB CG	LEU	235 235	23.294 -12.749 22.393 1.00 0.00	3A4
MOTA MOTA	1486		LEU	235	23.236 -11.785 23.594 1.00 0.00	3A4
MOTA	1487		LEU	235	22.289 -13.903 22.600 1.00 0.00	3A4 3A4
ATOM	1488	C	LEU	235	24.592 -13.413	3A4
ATOM	1489	0	LEU ASN	235 236	24.703 -14.586	3A4
ATOM ATOM	1490 1491	N CA	ASN	236	27.013 -13.135 19.089 1.00 0.00	3A4
ATOM	1492	CB	ASN	236	27.351 -13.966 17.803 1.00 0.00	3A4
ATOM	1493	CG	ASN	236	28.697 -14.706 17.931 1.00 0.00 28.818 -15.613 18.753 1.00 0.00	3A4 3A4
ATOM	1494		ASN	236	28.818 -15.613 18.753 1.00 0.00 29.719 -14.326 17.115 1.00 0.00	3A4
ATOM ATOM	1495 1496	C ND2	ASN ASN	236 236	27.795 -11.845 19.165 1.00 0.00	3A4
ATOM	1497	ŏ	ASN	236	28.546 -11.489 18.259 1.00 0.00	3A4
ATOM	1498	N	ILE	237	27.590 -11.096 20.283 1.00 0.00 28.074 -9.747 20.504 1.00 0.00	3A4 3A4
ATOM	1499	CA	ILE	237	28.074 -9.747 20.504 1.00 0.00 26.980 -8.800 20.998 1.00 0.00	3A4
MOTA MOTA	1500 1501	CB CG2	ILE ILE	237 237	26.039 -8.584 19.789 1.00 0.00	3A4
ATOM	1502		ILE	237	26.203 -9.271 22.262 1.00 0.00	3A4
ATOM	1503	CD	ILE	237	25.059 -8.341 22.671 1.00 0.00	3A4 3A4
ATOM	1504	C	ILE	237	29.228 -9.798 21.461 1.00 0.00 30.202 -9.126 21.226 1.00 0.00	3A4
ATOM	1505 1506	O N	ILE CYS	237 238	29.124 -10.614 22.532 1.00 0.00	3A4
MOTA MOTA	1507	CA	CYS	238	30.099 -10.834 23.576 1.00 0.00	3A4
ATOM	1508	СВ	CYS	238	29.513 -11.689 24.739 1.00 0.00	3A4 3A4
MOTA	1509	SG	CYS	238	28.106 -10.870	3A4
ATOM	1510	c o	CYS CYS	238 238	31.307 -11.563 23.083 1.00 0.00 32.424 -11.278 23.493 1.00 0.00	3A4
ATOM ATOM	1511 1512	N	VAL	239	31.138 -12.446 22.082 1.00 0.00	3A4
ATOM	1513	CA	VAL	239	32.219 -13.161 21.438 1.00 0.00	3A4
ATOM	1514	CB.	VAL	239	31.700 -14.367 20.675 1.00 0.00 32.858 -15.308 20.247 1.00 0.00	3A4 3A4
ATOM	1515		VAL	239 239	32.858 -15.308	3A4
ATOM ATOM	1516 1517	C	VAL	239	33.006 -12.283 20.505 1.00 0.00	3A4
ATOM	1518	ō	VAL	239	34.228 -12.327 20.485 1.00 0.00	3A.4
ATOM	1519	N	PHE	240	32.315 -11.420 19.731 1.00 0.00 32.913 -10.422 18.870 1.00 0.00	3A4 3A4
ATOM	1520 1521	CA CB	PHE	240 240	32.913 -10.422 18.870 1.00 0.00 31.825 -9.669 18.040 1.00 0.00	3A4
ATOM ATOM	1521	CG	PHE	240	31.881 -8.134 17.899 1.00 0.00	3A4
ATOM	1523		PHE	240	32.913 -7.550 17.149 1.00 0.00	3A4
MOTA	1524		PHE	240	31.185 -7.320 18.812 1.00 0.00 33.312 -6.223 17.382 1.00 0.00	3A4 3A4
MOTA	1525		PHE	240 240	33.312 -6.223 17.382 1.00 0.00 31.646 -6.034 19.117 1.00 0.00	3A4
MOTA MOTA	1526 1527	CZ	PHE !	240	32.709 -5.481 18.396 1.00 0.00	3A4
ATOM	1528	c	PHE	240	33.789 -9.440 19.608 1.00 0.00	3A4
MOTA	1529	0	PHE	240	34.906 -9.202 19.168 1.00 0.00 33.347 -8.835 20.727 1.00 0.00	3A4 3A4
ATOM	1530	N	PRO	241	33.347 -8.835 20.727 1.00 0.00 34.111 -7.940 21.493 1.00 0.00	3A4
MOTA MOTA	1531 1532	CA	PRO PRO	241 241	32.648 -9.345 21.724 1.00 0.00	3A4
ATOM	1532	СВ	PRO	241	33.196 -7.358 22.578 1.00 0.00	3A4
ATOM	1534	CG	PRO	241	32.348 -8.435 22.936 1.00 0.00	3A4 3A4
ATOM	1535	C	PRO		35.347 -8.605 22.103 1.00 0.00 36.396 -7.992 22.029 1.00 0.00	3A4
MOTA MOTA	1536 1537	O N	PRO ARG	241 242	35.316 -9.867 22.592 1.00 0.00	3A4
ATOM	1537	CA	ARG	242	36.450 -10.583 23.101 1.00 0.00	3A4
ATOM	1539		ARG	242	35.986 -11.889 23.750 1.00 0.00	3A4 3A4
MOTA	1540	CG	ARG		35.213 -11.657 25.054 1.00 0.00 34.515 -12.928 25.556 1.00 0.00	3A4
MOTA	1541	CD	ARG	242	34.515 -12.928 25.556 1.00 0.00	

ATOM	1542	NE	ARG	242	33.717 -	12.581	26.784	1.00	0.00	3A4
ATOM	1543	CZ	ARG	242	32.762 -		27.314	1.00	0.00	3A4
ATOM	1544	NH1.	ARG	242	32.114 -		28.455	1.00	0.00	3A4
MOTA	1545	NH2		242	32.444 -		26.725	1.00	0.00 0.00	3A4 3A4
MOTA	1546	C	ARG	242	37.483 -		22.037 22.298	1.00	0.00	3A4
MOTA	1547	0	ARG	242 243	38.677 - 37.044 -		20.784	1.00	0.00	3A4
MOTA MOTA	1548 1549	N CA	GLU	243	37.911 -		19.638	1.00	0.00	3A4
ATOM	1550	СВ	GLU	243	37.126 -		18.383	1.00	0.00	3A4
ATOM	1551	CG	GLU	243	36.626 -	13.298	18.452	1.00	0.00	3A4
ATOM	1552	CD	GLU	243	35.759 -		17.219	1.00	0.00	3A4 3A4
ATOM	1553		GLU	243	34.528 - 36.319 -		17.385 16.089	1.00	0.00	3A4
ATOM	1554		GLU GLU	243 243	38.703 -		19.275	1.00	0.00	3A4
MOTA MOTA	1555 1556	С 0	GLU	243	39.908 -		19.057	1.00	0.00	3A4
ATOM	1557	N	VAL	244	38.043	-8.981	19.287	1.00	0.00	3A4
ATOM	1558	CA	VAL	244	38.684	-7.714	18.990	1.00	0.00	3A4 3A4
MOTA	1559	СВ	VAL	244	37.676	-6.607	18.731	1.00	0.00	· 3A4
ATOM	1560		VAL	244	38.391 36.813	-5.314 -7.052	18.259 17.545	1.00	0.00	3A4
MOTA MOTA	1561 1562	CG2 C	VAL VAL	244 244	39.649	-7.327	20.084	1.00	0.00	3A4
ATOM	1563	ō	VAL	244	40.771	-6.912	19.811	1.00	0.00	3A4
ATOM	1564	N	THR	245	39.257	-7.535	21.357	1.00	0.00	3A4
MOTA	1565	CA	THR	245	40.070	-7.264	22.527	1.00	0.00	3A4 3A4
ATOM	1566	СВ	THR	245	39.245	-7.434	23.795 23.817	1.00 1.00	0.00	3A4
MOTA	1567		THR THR	245 245	38.211 40.041	-6.455 -7.330	25.127	1.00	0.00	3A4
MOTA MOTA	1568 1569	C	THR	245	41.317	-8.113	22.572	1.00	0.00	3A4
ATOM	1570	ō	THR	245	42.397	-7.605	22.842	1.00	0.00	3A4
MOTA	1571	N	ASN	246	41.225	-9.408	22.207	1.00	0.00	3A4 3A4
MOTA	1572	CA	ASN	246	42.344		22.152 21.874	1.00	0.00 0.00	3A4
ATOM	1573	CB	ASN	246 246	41.877 - 41.116 -		23.082	1.00	0.00	3A4
MOTA MOTA	1574 1575	CG	ASN ASN	246	41.128		24.187	1.00	0.00	3A4
ATOM	1576		ASN	246	40.427	-13.502	22.862	1.00	0.00	3A4
MOTA	1577	С	ASN	246	43.340		21.088	1.00	0.00	3A4
MOTA	1578	0	ASN	246		-10.003	21.305	1.00	0.00	3A4 3A4
MOTA	1579	N	PHE	247	42.846 43.640	-9.491 -9.006	19.921 18.820	1.00	0.00	3A4
ATOM ATOM	1580 1581	CA CB	PHE	247 247	42.712	-8.691	17.625	1.00	0.00	3A4
ATOM	1582	CG	PHE	247	43.520	-8.335	16.378	1.00	0.00	3A4
ATOM	1583		PHE	247	44.084	-9.348	15.580	1.00	0.00	3A4 3A4
MOTA	1584		PHE		43.817	-6.990	16.065	1.00	0.00	3A4
ATOM	1585	CEI		247	44.943 44.673	-9.028 -6.665	14.517 15.008	1.00	0.00	3A4
ATOM	1586 1587	CE2	PHE	247 247	45.245	-7.686	14.243	1.00	0.00	3A4
MOTA MOTA	1588	c	PHE	247	44.438	-7.768	19.171	1.00	0.00	3A4
ATOM	1589	o	PHE	247	45.631	-7.693	18.897	1.00	0.00	3A4
MOTA	1590	N	LEU	248	43.781	-6.766	19.795	1.00	0.00	. 3A4 3A4
MOTA	1591	CA	LEU	248	44.374 43.291	-5.480 -4.473	20.131 20.599	1.00	0.00	3A4
ATOM	1592 1593	CB CG	LEU	248 248	42.423	-3.985	19.422	1.00	0.00	3A4
MOTA MOTA	1594		LEU	248	41.143	-3.318	19.920	1.00	0.00	3A4
ATOM	1595		LEU	248	43.179	-3.055	18.448	1.00	0.00	3A4
MOTA	1596	С	LEU	248	45.407	-5.587	21.219	1.00	0.00	3A4 3A4
MOTA	1597	0	LEU	248	46.458	-4.959 -6.483	21.175 22.189	1.00	0.00	3A4
ATOM ATOM	1598 1599	N CA	ARG ARG	249 249	45.152 46.055	-6.805	23.263	1.00	0.00	3A4
MOTA	1600	CB	ARG	249	45.402	-7.886	24.160	1.00	0.00	3A4
MOTA	1601	CG	ARG	249	44.526	-7.297	25.274	1.00	0.00	3A4
ATOM	1602	CD	ARG	249	45.372	-6.731	26.426		0.00	3A4 3A4
MOTA	1603	NE	ARG	249	44.462	-6.210 -5.795	27.502 28.722		0.00	3A4
ATOM	1604	CZ	ARG L ARG	249 249	44.932 44.068	-5.248	29.621			3A4
MOTA MOTA	1605 1606		ARG		46.251	-5.917	29.056		0.00	3A4
ATOM	1607	C	ARG		47.418	-7.301	22.846	1.00		3A4
ATOM	1608	ŏ	ARG	249	48.444	-6.897	23.385			3A4 3A4
ATOM	1609	N	LYS		47.456	-8.139	21.790			3A4 3A4
ATOM	1610	CA	LYS		48.664 48.353	-8.643 -9.760	21.183			3A4
ATOM	1611	CB CG	LYS LYS			-11.007	20.790			3A4
MOTA MOTA	1612 1613	CD		_	47.184	-11.995	19.759			3A4
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	ATOH	1614	CE	LYS	250	46.472	-13.190	20.404	1.00	0.00	3A4
	ATOM	1615	NZ	LYS	250	45.925	-14.102	19.372	1.00	0.00	3A4
	ATOM	1616	С	LYS	250	49.481	-7.572	20.506	1.00	0.00	3A4
	MOTA	1617	Ó	LYS	250	50.699	-7.572	20.583	1.00	0.00	3A4 3A4
	ATOM	1618	N	SER	251	48.809 49.413	-6.584 -5.423	19.881 19.268	1.00	0.00	3A4
	ATOM	1619	CA CB	SER SER	251 251	48.350	-4.598	18.498	1.00	0.00	3A4
	ATOM ATOM	1620 1621	OG	SER	251	47.705	-5.410	17.524	1.00	0.00	3A4
	ATOM	1622	c	SER	251	50.056	-4.492	20.271	1.00	0.00	3A4
	ATOM	1623	0	SER	251	51.163	-4.000	20.091	1.00	0.00	3A4
	ATOM	1624	N	VAL	252	49.376	-4.275	21.416	1.00	0.00	3A4 3A4
	ATOM	1625	CA	VAL	252	49.809	-3.398 -3.198	22.495 23.486	1.00	0.00	3A4
	ATOM	1626 1627	CB	VAL VAL	252 252	48.673 49.132	-2.497	24.775	1.00	0.00	3A4
	ATOM ATOM	1628		VAL	252	47.610	-2.462	22.625	1.00	0.00	3A4
	ATOM	1629	c	VAL	252	51.052	-3.938	23.163	1.00	0.00	3A4
	ATOM	1630	0	VAL	252	51.998	-3.206	23.419	1.00	0.00	3A4
	ATOM	1631	N	LYS	253	51.108		23.380	1.00	0.00	3A4 3A4
	ATOM	1632	CA	LYS	253	52.243	-5.976 -7.462	23.944 24.155	1.00 1.00	0.00	3A4
	ATOM	1633	CB	LYS	253 253	51.887 52.903	-8.297	24.153	1.00	0.00	3A4
	ATOM ATOM	1634 1635	CG CD	LYS LYS	253 253	52.410	-9.721	25.224	1.00	0.00	3A4
	ATOM	1636	ÇE	LYS	253		-10.563	26.018	1.00	0.00	3A4
	ATOM	1637	NZ	LYS	253	52.893	-11.929	26.256	1.00	0.00	3A4
	ATOM	1638	С	LYS	253	53.481	-5.877	23.082	1.00	0.00	3A4
	MOTA	1639	0	LYS	253	54.570	-5.578	23.557	1.00	0.00	3A4 3A4
	ATOM	1640	N	ARG	254	53.316 54.372	-6.057 -5.928	21.752 20.768	1.00	0.00	3A4
	ATOM	1641 1642	CA CB	ARG ARG	254 254	53.887	-6.368	19.369	1.00	0.00	3A4
	ATOM ATOM	1643	CG	ARG	254	53.631	-7.877	19.278	1.00	0.00	3A4
	ATOM	1644	CD	ARG	254	52.822	-8.252	18.031	1.00	0.00	3A4
	ATOM	1645	NE	ARG	254	52.473	-9.714	18.098	1.00	0.00	3A4
	MOTA	1646	CZ	ARG	254		-10.256	17.466	1.00	0.00	3A4 3A4
	MOTA	1647		ARG	254	51.133	-11.591 -9.490	17.596 16.721	1.00	0.00 0.00	3A4
	ATOM	1648 1649		ARG ARG	254 254	54.899	-4.517	20.676	1.00	0.00	3A4
	ATOM ATOM	1650	0	ARG	254	56.093	-4.310	20.498	1.00	0.00	3A4
	ATOM	1651	N	MET		54.021	-3.508	20.844	1.00	0.00	3A4
	ATOM	1652	CA	MET	255	54.372	-2.106	20.777	1.00	0.00	3A4
	MOTA	1653	CB	MET	255	53.141	-1.258	20.406	1.00	0.00	3A4 3A4
	ATOM	1654	CG	MET	255	52.816	-1.403 -0.639	18.917 18.447	1.00	0.00	3A4
	ATOM	1655 1656	SD CE	MET MET	255 255	51.250 51.470		16.649	1.00	0.00	3A4
	ATOM ATOM	1657	C	MET	255	55.008		22.041	1.00	0.00	3A4
•	ATOM	1658	ŏ	MET	255	55.687	-0.563	22.027	1.00	0.00	3A4
	MOTA	1659	N	LYS	256	54.853		23.174	1.00	0.00	3A4
	MOTA	1660	CA	LYS	256	55.524	-1.998	24.424	1.00	0.00	3A4 3A4
	ATOM	1661	CB	LYS	256	54.809 53.537		25.623 26.076	1.00	0.00 0.00	3A4
	ATOM ATOM	1662 1663	CD CD	LYS LYS	256 256	52.726		27.168	1.00	0.00	3A4
	ATOM	1664	CE	LYS	256	53.383		28.556	1.00	0.00	3A4
	ATOM	1665	NZ	LYS	256	52.487		29.579	1.00	0.00	3A4
	MOTA	1666	С	LYS	256	56.960		24.397	1.00	0.00	3A4
	MOTA	1667	0	LYS	256	57.837		25.029		0.00	3A4 3A4
	MOTA	1668	N	GLU	257	57.220 58.527		23.619 23.444	1.00	0.00	3A4
	MOTA MOTA	1669 1670	CA CB	GLU GLU	257 257	58.421		23.058	1.00	0.00	3A4
	ATOM	1671	CG	GLU	257	57.813		24.182	1.00	0.00	3A4
	ATOM	1672	CD	GLU	257	57.607	-7.953	23.679	1.00	0.00	3A4
	ATOM	1673	OE1	GLU	257	56.428		23.604	1.00	0.00	3A4
	MOTA	1674		GLU	257	58.625		23.363	1.00	0.00	3A4 3A4
	ATOM	1675	C	GLU	257 257	59.381 60.407		22.410 22.760	1.00	0.00	3A4
	ATOM ATOM	1676 1677	O N	GLU SER	257 258	59.003		21.108	1.00	0.00	3A4
	ATOM	1678	CA	SER	258	59.766		20.026	1.00	0.00	3A4
	ATOM	1679	СВ	SER	258	61.186	-3.589	19.807	1.00	0.00	3A4
	ATOM	1680	OG	SER	258	62.002		18.899	1.00	0.00	3A4
	ATOM	1681	С	SER	258	58.938		18.776		0.00	3A4 3A4
	ATOM	1682	0	SER	258 250	58.503 58.779		18.459 18.007	1.00	0.00	3A4
	ATOM ATOM	1683 1684	N CA	ARG ARG	259 259	58.391		16.612		0.00	3A4
	ATOM	1685	CB	ARG	259	56.880		16.329		0.00	3A4

ATOM	1686	CG	ARG	259	55.968	-2.939	16.688	1.00	0.00	3A4
ATOM	1687	CD	ARG	259	54.607	-2.858	15.987	1.00	0.00	3A4
ATOM	1688	NE	ARG	259	53.744	-4.000	16.458	1.00	0.00	3A4
ATOM	1689	CZ	ARG	259	52.617	-4.411	15.791	1.00	0.00	3A4
ATOM	1690	NH1		259	51.837	-5.390	16.332	1.00	0.00	3A4
ATOM	1691	NH2		259	52.247	-3.859	14.598	1.00	0.00	3A4
ATOM	1692	С	ARG	259	59.262	-0.943	16.000	1.00	0.00	3A4
ATOM	1693	ō	ARG	259	60.401	-1.220	15.626	1.00	0.00	3A4
MOTA	1694	N	LEU	260	58.752	0.314	15.898	1.00	0.00	3A4
ATOM	1695	CA	LEU	260	59.502	1.436	15.373	1.00	0.00	3A4
ATOM	1696	CB	LEU	260	59.602	1.425	13.811	1.00	0.00	3A4
ATOM	1697	CG	LEU	260	60.595	2.428	13.175	1.00	0.00	3A4
ATOM	1698	CD1		260	62.054	2.163	13.599	1.00	0.00	3A4
ATOM	1699	CD2		260	60.467	2.427	11.640	1.00	0.00	3A4
MOTA	1700	С	LEU	260	58.790	2.670	15.874	1.00	0.00	3A4
ATOM	1701	0	LEU	260	58.005	3.291	15.159	1.00	0.00	3A4
ATOM	1702	N	GLU	261	59.062	3.038	17.155	1.00	0.00	3A4
MOTA	1703	CA	GLU	261	58.441	4.130	17.884	1.00	0.00	3A4
ATOM	1704	CB	GLU	261	57.742	3.683	19.213	1.00	0.00	3A4
MOTA	1705	CG	GLU	261	58.554	2.841	20.229	1.00	0.00	3A4
ATOM	1706	CD	GLU	261	58.717	1.386	19.761	1.00	0.00	3A4
MOTA	1707	OE1	GLU	261	59.884	0.942	19.589	1.00	0.00	. 3A4
ATOM	1708	OE2	GLU	261	57.675	0.701	19.572	1.00	0.00	3A4
ATOM	1709	С	GLU	261	59.482	5.186	18.166	1.00	0.00	3A4
ATOM	1710	0	GLU	261	60.619	4.877	18.523	1.00	0.00	3A4
MOTA	1711	N	ASP	262	59.067	6.478	17.991	1.00	0.00	3A4
ATOM	1712	CA	ASP	262	59.771	7.738	18.239	1.00	0.00	3A4
ATOM	1713	CB	ASP	262	60.392	7.859	19.674	1.00	0.00	3A4
ATOM	1714	CG	ASP	262	59.293	7.671	20.735	1.00	0.00	3A4
ATOM	1715	OD1	ASP	262	59.392	6.700	21.533	1.00	0.00	3A4
ATOM	1716	OD2	ASP	262	58.341	8.497	20.759	1.00	0.00	3A4 3A4
ATOM	1717	С	ASP	262	60.828	8.011	17.175	1.00	0.00	3A4
ATOM	1718	0	ASP	262	62.015	8.125	17.477	1.00	0.00	3A4
ATOM	1719	Ν.	THR	263	60.385	8.087	15.889	1.00	0.00 0.00	3A4
ATOM	1720	CA	THR	263	61.231	8.151	14.709	1.00	0.00	3A4
ATOM	1721	CB	THR	263	61.257	6.828	13.922	1.00	0.00	3A4
MOTA	1722		THR	263	59.962	6.247	13.768	1.00	0.00	3A4
ATOM	1723	CG2		263	62.163	5.831	14.677	1.00	0.00	3A4
MOTA	1724	C	THR	263	60.819	9.346	14.127	1.00	0.00	3A4
ATOM	1725	0	THR	263	61.248	10.466 9.120	12.773	1.00	0.00	3A4
MOTA	1726	N	GLN	264	60.017 59.831	10.032	11.649	1.00	0.00	3A4
MOTA	1727	CA	GLN	264	59.812	9.263	10.288	1.00	0.00	3A4
MOTA	1728	CB	GLN	264	61.018	8.324	10.094	1.00	0.00	3A4
MOTA	1729	CG	GLN	264 264	60.951	7.671	8.710	1.00	0.00	3A4
MOTA	1730	CD	GLN	264	61.775	7.968	7.846	1.00	0.00	3A4
MOTA	1731	OE1	GLN GLN	264	59.961	6.763	8.489	1.00	0.00	3A4
ATOM	1732 1733	Ç	GLN	264	58.564	10.861	11.768	1.00	0.00	3A4
ATOM	1734	ò	GLN	264	57.907	10.891	12.808	1.00	0.00	3A4
ATOM ATOM	1735	N	LYS	265	58.214	11.556	10.645	1.00	0.00	3A4
ATOM	1736	CA	LYS	265	57.091	12.459	10.453	1.00	0.00	3A4
ATOM	1737	СВ	LYS	265	57.471	13.608	9.470	1.00	0.00	3A4
ATOM	1738	CG	LYS	265	56.414	14.703	9.209	1.00	0.00	3A4
ATOM	1739	CD	LYS	265	55.986	15.485	10.458	1.00	0.00	3A4
ATOM	1740	CE	LYS	265	55.004	16.618	10.140	1.00	0.00	3A4
ATOM	1741	NZ	LYS	265	54.585	17.323	11.374	1.00	0.00	3A4
ATOM	1742	C	LYS	265	55.895	11.698	9.920	1.00	0.00	3A4
ATOM	1743	ō	LYS	265	54.757	11.957	10.308	1.00	0.00	3A4
ATOM	1744	N	HIS	266	56.161	10.712	9.017	1.00	0.00	3A4
ATOM	1745	CA	HIS	266	55.192	9.789	8.453	1.00	0.00	3A4
ATOM	1746		HIS	266	53.213	11.484	6.555	1.00	0.00	3A4
ATOM	1747	CG	HIS	266	54.551	11.168	6.457	1.00	0.00	3A4
ATOM	1748	СВ	HIS	266	55.138	9.857	6.906		0.00	3A4
ATOM	1749		HIS	266	54.234	13.294	5.769	1.00	0.00	3A4
MOTA	1750		HIS	266	55.161	12.287	5.977		0.00	3A4
ATOM	1751		HIS	266	53.080	12.764	6.128		0.00	3A4
MOTA	1752	C	HIS	266	55.520	8.402	8.961			3A4
ATOM	1753	Ó	HIS	266	55.595	7.432	8.208			3A4
ATOM	1754	N	ARG	267	55.681	8.319	10.306			3A4
ATOM	1755	CA	ARG	267	55.787	7.112	11.088			3A4
ATOM	1756	СВ	ARG		57.206	6.450	11.025			3A4
ATOM	1757	CG	ARG	267	57.342	5.024	11.602	1.00	0.00	3A4

ATOM	1758	CD	ARG	267	56.433	3.983	10.915	1.00	0.00	3A4
ATOM	1759	NE	ARG	267	56.515	2.666	11.644	1.00	0.00	3A4
ATOM	1760	CZ	ARG	267	55.718	2.342	12.715	1.00	0.00	3A4
ATOM	1761		ARG	267	55.829	1.104	13.280	1.00	0.00	3A4
ATOM	1762		ARG	267	54.819	3.229	13.235	1.00	0.00	3A4
ATOM	1763	C	ARG	267	55.443	7.575	12.488	1.00	0.00	3A4
ATOM	1764	ŏ	ARG	267	55.403	8.776	12.757	1.00	0.00	3A4
ATOM	1765	N	VAL	268	55.180	6.600	13.409	1.00	0.00	3A4
ATOM	1766	CA	VAL	268	54.850	6.700	14.830	1.00	0.00	3A4
ATOM	1767	СВ	VAL	268	55.608	7.738	15.672	1.00	0.00	3A4
ATOM	1768		VAL	268	55.286	7.564	17.181	1.00	0.00	3A4
ATOM	1769		VAL	268	57.124	7.555	15.459	1.00	0.00	3A4
ATOM	1770	C	VAL	268	53.347	6.859	14.949	1.00	0.00	3A4
ATOM	1771	ō	VAL	268	52.814	7.966	14.876	1.00	0.00	3A4
ATOM	1772	N	ASP	269	52.650	5.703	15.128	1.00	0.00	3A4
ATOM	1773	CA	ASP	269	51.217	5.484	15.039	1.00	0.00	3A4
ATOM	1774	СВ	ASP	269	50.952	4.008	14.629	1.00	0.00	3A4
ATOM	1775	CG	ASP	269	51.584	2.963	15.562	1.00	0.00	3A4
ATOM	1776	OD1	ASP	269	52.585	2.329	15.136	1.00	0.00	3A4
ATOM	1777	OD2	ASP	269	51.040	2.734	16.671	1.00	0.00	3A4
ATOM	1778	С	ASP	269	50.513	5.855	16.322	1.00	0.00	3A4
ATOM	1779	0	ASP	269	51.163	6.144	17.324	1.00	0.00	3A4
ATOM	1780	N	PHE	270	49.161	5.834	16.331	1.00	0.00	3A4
ATOM	1781	CA	PHE	270	48.362	6.204	17.490	1.00	0.00	3A4
ATOM	1782	СВ	PHE	270	46.855	6.258	17.148	1.00	0.00	3A4
ATOM	1783	CG	PHE	270	45.990	6.766	18.282	1.00	0.00	3A4
ATOM	1784	CD1	PHE	270	45.280	5.854	19.081	1.00	0.00	3A4
ATOM	1785	CD2	PHE	270	46.020	8.114	18.661	1.00	0.00	3A4
MOTA	1786	CE1	PHE	270	44.531	6.282	20.177	1.00	0.00	3A4
ATOM	1787	CE2	PHE	270	45.309	8.546	19.789	1.00	0.00	3A4
ATOM	1788	CZ	PHE	270	44.542	7.634	20.522	1.00	0.00	3A4
ATOM	1789	С	PHE	270	48.565	5.305	18.696	1.00	0.00	3A4
ATOM	1790	0	PHE	270	48.623	5.789	19.822	1.00	0.00	3A4
MOTA	1791	N	LEU	271	48.707	3.980	18.488	1.00	0.00	3A4
ATOM	1792	CA	LEU	271	48.911	3.039	19.569	1.00	0.00	3A4
ATOM	1793	СВ	LEU	271	48.798	1.584	19.058	1.00	0.00	3A4
MOTA	1794	CG	LEU	271	47.377	1.034	18.852	1.00	0.00	3A4
ATOM	1795	CD1	LEU	271	47.422	-0.399	18.277	1.00	0.00	3A4
ATOM	1796	CD2	LEU	271	46.550	1.035	20.150	1.00	0.00	3A4
MOTA	1797	С	LEU	271	50.247	3.247	20.287	1.00	0.00	3A4
MOTA	1798	0	LEU	271	50.309	3.283	21.510	1.00	0.00	3A4
ATOM	1799	N	GLN	272	51.325	3.513	19.518	1.00	0.00	3A4
MOTA	1800	CA	GLN	272	52.641	3.856	20.018	1.00	0.00	3A4
ATOM	1801	СВ	GLN	272	53.651	3.973	18.871	1.00	0.00	3A4
ATOM	1802	CG	GLN	272	53.989	2.568	18.334	1.00	0.00	3A4
MOTA	1803	CD	GLN	272	54.908	2.656	17.119	1.00	0.00	3A4
MOTA	1804	OE 1		272	55.225	3.735	16.626		0.00	3A4
ATOM	1805	NE2		272	55.347	1.475	16.611	1.00	0.00	3A4
ATOM	1806	С	GLN	272	52.646	5.136	20.813	1.00	0.00	3A4
ATOM	1807	0	GLN	272	53.254	5.214	21.874	1.00	0.00	3A4
ATOM	1808	N	LEU	273	51.883	6.155	20.356	1.00	0.00	3A4
ATOM	1809	CA	LEU	273	51.695	7.415	21.048	1.00	0.00	3A4
ATOM	1810	СВ	LEU	273	50.926	8.433	20.166	1.00	0.00	3A4
ATOM	1811	CG	LEU	273	51.785	8.888	18.948	1.00	0.00	3A4 3A4
MOTA	1812	CD1		273	50.959	9.439	17.771	1.00		
MOTA	1813	CD2		273	52.899	9.882	19.332	1.00	0.00	3A4 3A4
MOTA	1814	C	LEU	273	50.983	7.274	22.346 23.329	1.00	0.00	3A4
MOTA	1815	0	LEU	273	51.365	7.895	23.329	1.00		3A4
ATOM	1816	N	MET	274	49.964	6.395		1.00	0.00	3A4
MOTA	1817	CA	MET	274	49.244	6.073	23.621		0.00	
ATOM	1818	CB	MET	274	47.977	5.254	23.316	1.00	0.00	3A4 3A4
ATOM	1819	CG	MET	274	46.828	6.090	22.751	1.00	0.00	3A4
ATOM	1820	SD	MET	274	45.317	6.067	23.770	1.00	0.00	3A4
ATOM	1821	CE	MET	274	45.991 50 100	6.940	25.218 24.619	1.00	0.00	3A4
ATOM	1822	C	MET	274	50.109 50.038	5.325 5.567	25.819	1.00	0.00	3A4
ATOM	1823	0	MET	274	50.038	4.417	24.131	1.00	0.00	3A4
ATOM	1824	N	ILE	275 275			24.131	1.00	0.00	3A4
MOTA	1825	CA	ILE	275	51.851 52.467	3.564	24.931	1.00	0.00	3A4
ATOM	1826	CB	ILE	275	52.467 53.965	2.441 2.545	23.648	1.00	0.00	3A4
ATOM	1827 1828		ILE	275 275	53.965 52.209	1.038	24.643	1.00	0.00	3A4
ATOM ATOM	1828	CD	ILE	275 275	51.787	0.081	23.536	1.00	0.00	3A4
AION	1023	CD	100	2/3	31.707	0.061	23.330	1.00	5.00	~1

ATOM	1830	С	ILE	275	52.925	4.329	25.660	1.00	0.00	3A4
ATOM	1831	ō	ILE	275	53.323	3.975	26.764	1.00	0.00	3A4
ATOM	1832	N	ASP	276	53.392	5.425	25.033	1.00	0.00	3A4
ATOM	1833	CA	ASP	276	54.488	6.233	25.491	1.00	0.00	3A4
ATOM	1834	СВ	ASP	276	55.375	6.635	24.263	1.00	0.00	3A4
ATOM	1835	CG	ASP	276	56.766	7.177	24.648	1.00	0.00	3A4
ATOM	1836	OD1		276	57.527	6.432	25.323	1.00	0.00	3A4
ATOM	1837	OD2		276	57.080	8.336	24.266	1.00	0.00	3A4
ATOM	1838	С	ASP	276	53.994	7.467	26.229	1.00	0.00	3A4
MOTA	1839	0	ASP	276	54.738	8.023	27.029	1.00	0.00	3A4
MOTA	1840	N	SER	277	52.734	7.918	25.959	1.00	0.00	3A4
ATOM	1841	CA	SER	277	51.962	9.005	26.574	1.00	0.00	3A4
ATOM	1842	CB	SER	277	51.494	8.689	28.034	1.00	0.00	3A4
ATOM	1843	OG	SER	277	52.536	8.498	28.989	1.00	0.00	3A4
ATOM	1844	С	SER	277	52.586	10.401	26.477	1.00	0.00	3A4
MOTA	1845	0	SER	277	53.547	10.719	27.177	1.00	0.00	3A4
ATOM	1846	N	GLN	278	52.027	11.259	25.584	1.00	0.00	3A4
ATOM	1847	CA	GLN	278	52.576	12.557	25.230	1.00	0.00	3A4
MOTA	1848	CB	GLN	278	53.079	12.585	23.748	1.00	0.00	3A4
ATOM	1849	ÇG	GLN	278	52.289	11.752	22.708	1.00	0.00	3A4
ATOM	1850	CD	GLN	278	50.896	12.317	22.436	1.00	0.00	3A4
ATOM	1851	OE1		278	49.896	11.703	22.807	1.00	0.00	3A4
MOTA	1852	NE2		278	50.821	13.500	21.767	1.00	0.00	3A4 3A4
MOTA	1853	С	GLN	278	51.568	13.647	25.534	1.00	0.00	3A4
ATOM	1854	0	GLN	278	51.306	14.524	24.712	1.00	0.00	3A4
ATOM	1855	N	ASN	279	51.016	13.632	26.775	1.00	0.00	3A4
MOTA	1856	CA	ASN	279	50.193	14.697	27.310	1.00	0.00	3A4
ATOM	1857	СВ	ASN	279	48.716	14.690	26.781 27.107	1.00	0.00	3A4
ATOM	1858	CG	ASN	279	47.973	15.999	28.136	1.00	0.00	3A4
ATOM	1859	OD1		279	47.305 48.086	16.089 17.026	26.221	1.00	0.00	3A4
ATOM	1860	ND2		279 279	50.239	14.505	28.808	1.00	0.00	3A4
ATOM	1861	C	ASN ASN	279	50.626	15.409	29.546	1.00	0.00	3A4
ATOM ATOM	1862 1863	O N	SER	280	49.821	13.295	29.277	1.00	0.00	3A4
ATOM	1864	CA	SER	280	49.736	12.901	30.674	1.00	0.00	3A4
ATOM	1865	CB	SER	280	48.334	12.330	31.056	1.00	0.00	3A4
ATOM	1866	OG	SER	280	47.313	13.268	30.740	1.00	0.00	3A4
ATOM	1867	c	SER	280	50.810	11.870	30.942	1.00	0.00	3A4
ATOM	1868	ō	SER	280	51.635	11.569	30.079	1.00	0.00	3A4
ATOM	1869	N	LYS	281	50.813	11.317	32.183	1.00	0.00	3A4
ATOM	1870	CA	LYS	281	51.810	10.412	32.724	1.00	0.00	3A4
ATOM	1871	СВ	LYS	281	52.318	10.863	34.135	1.00	0.00	3A4
MOTA	1872	CG	LYS	281	51.368	10.740	35.357	1.00	0.00	3A4
ATOM	1873	CD	LYS	281	50.099	11.612	35.328	1.00	0.00	3A4
MOTA	1874	CE	LYS	281	49.241	11.508	36.598	1.00	0.00	3A4
ATOM	1875	NZ	LYS	281	48.695	10.139	36.770	1.00	0.00	3A4
MOTA	1876	С	LYS	281	51.259	9.009	32.800	1.00	0.00	3A4
ATOM	1877	0	LYS	281	50.051	8.792	32.725	1.00	0.00	3A4
MOTA	1878	N	GLU	282	52.179	.8.025	33.003	1.00	0.00	. 3A4
ATOM	1879	CA	GLU	282	51.902	6.623	33.252	1.00	0.00	3A4 3A4
MOTA	1880	СВ	GLU	282	52.839	5.684	32.439	1.00	0.00	3A4
MOTA	1881	CG	GLU	282	54.355 55.125	5.905	32.633	1.00	0.00	3A4
MOTA	1882	CD	GLU	282	54.983	5.055 5.322	31.617 30.393	1.00	0.00	3A4
MOTA	1883		GLU	282	55.866	4.133	32.049	1.00	0.00	3A4
ATOM	1884		GLU	282 282	52.026	6.378	34.739	1.00	0.00	3A4
ATOM	1885	c o	GLU GLU	282	52.842	7.002	35.416	1.00	0.00	3A4
ATOM	1886 1887	и	THR	283	51.169	5.468	35.281	1.00	0.00	3A4
ATOM ATOM	1888	CA	THR	283	50.949	5.262	36.708	1.00	0.00	3A4
ATOM	1889	СВ	THR	283	49.462	5.076	37.037	1.00	0.00	3A4
ATOM	1890		THR	283	48.843	4.071	36.236	1.00	0.00	3A4
ATOM	1891		THR	283	48.746	6.425	36.797	1.00	0.00	3A4
ATOM	1892	C	THR	283	51.786	4.117	37.266	1.00	0.00	3A4
ATOM	1893	ŏ	THR	283	51.843	3.935	38.481	1.00	0.00	3A4
ATOM	1894	N	GLU	284	52.457	3.329	36.385	1.00	0.00	3A4
ATOM	1895	CA	GLU	284	53.336	2.253	36.792	1.00	0.00	3A4
ATOM	1896	СВ	GLU	284	52.583	0.907	37.025	1.00	0.00	3A4
ATOM	1897	CG	GLU	284	53.427	-0.211	37.670	1.00	0.00	3A4
ATOM	1898	CD	GLU	284	52.553	-1.452	37.873	1.00	0.00	3A4
MOTA	1899		GLU	284	52.075	-2.014	36.851	1.00	0.00	3A4
MOTA	1900	OE2	GLU	284	52.352	-1.855	39.051	1.00	0.00	3A4
MOTA	1901	С	GLU	284	54.393	2.152	35.719	1.00	0.00	3A4

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MOTA	1902	0	GLU	284	55.397	2.861	35.770	1.00	0.00	3A4
ATOM	1903	N	SER	285	54.186	1.256	34.721	1.00	0.00	3A4
ATOM	1904	CA	SER	285	55.139	0.973	33.669	1.00	0.00	3A4
MOTA	1905	CB	SER	285	56.281	-0.008	34.108	1.00	0.00	3A4
MOTA	1906	OG	SER	285	55.800	-1.171	34.781	1.00	0.00	3A4
MOTA	1907	С	SER	285	54.331	0.438	32.510	1.00	0.00	3A4
ATOM	1908	0	SER	285	54.522	-0.694	32.066	1.00	0.00	3A4
ATOM	1909	N	HIS	286	53.396	1.275	31.998	1.00	0.00	3A4 3A4
ATOM	1910	CA	HIS	286	52.522 49.824	0.926 1.672	30.901 32.816	1.00	0.00	3A4.
ATOM	1911	CG	HIS HIS	286 286	50.594	0.542	32.645	1.00	0.00	3A4
ATOM ATOM	1912 1913	СВ	HIS	286	51.264	0.113	31.356	1.00	0.00	3A4
ATOM	1914		HIS	286	49.782	0.592	34.753	1.00	0.00	3A4
ATOM	1915		HIS	286	50.557	-0.106	33.843	1.00	0.00	3A4
ATOM	1916		HIS	286	49.366	1.652	34.090	1.00	0.00	3A4
ATOM	1917	С	HIS	286	52.192	2.222	30.200	1.00	0.00	3A4
MOTA	1918	0	HIS	286	53.089	2.937	29.758	1.00	0.00	3A4
MOTA	1919	N	LYS	287	50.878	2.537	30.069	1.00	0.00	3A4
MOTA	1920	CA	LYS	287	50.317	3.652	29.338	1.00	0.00	3A4
MOTA	1921	CB	LYS	287	49.136	3.180	28.453	1.00	0.00	3A4
ATOM	1922	CG	LYS	287	49.553	2.209	27.349	1.00	0.00	3A4
ATOM	1923	CD	LYS	287	48.717	2.529	26.095	1.00	0.00	3A4 3A4
ATOM	1924	CE	LYS	287 287	48.931 47.885	1.795 2.079	24.736 23.732	1.00	0.00 0.00	3A4
ATOM	1925 1926	NZ C	LYS LYS	287	49.794	4.698	30.287	1.00	0.00	3A4
ATOM ATOM	1927	Ö	LYS	287	49.872	4.548	31.504	1.00	0.00	3A4
ATOM	1928	N	ALA	288	49.185	5.771	29.701	1.00	0.00	3A4
ATOM	1929	CA	ALA	288	48.374	6.783	30.350	1.00	0.00	3A4
ATOM	1930	СВ	ALA	288	48.615	8.202	29.810	1.00	0.00	3A4
ATOM	1931	С	ALA	288	46.906	6.403	30.192	1.00	0.00	3A4
MOTA	1932	0	ALA	288	46.333	6.618	29.125	1.00	0.00	3A4
MOTA	1933	И	LEU	289	46.245	5.810	31.226	1.00	0.00	3A4
ATOM	1934	CA	LEU	289	46.774	5.489	32.535	1.00	0.00	3A4
ATOM	1935	СВ	LEU	289	46.349	6.484	33.668	1.00	0.00	3A4
ATOM	1936	CG	LEU	289	44.839	6.740	33.920	1.00	0.00	3A4
ATOM	1937		LEU	289	44.604 44.221	7.179 7.776	35.378	1.00	0.00	3A4 3A4.
ATOM	1938		LEU	289 289	44.221	4.056	32.951 32.878	1.00	0.00	3A4.
ATOM ATOM	1939 1940	С О	LEU LEU	289	46.614	3.704	34.048	1.00	0.00	3A4
ATOM	1941	N	SER	290	46.131	3.176	31.880	1.00	0.00	3A4
ATOM	1942	CA	SER	290	46.112	1.765	32.148	1.00	0.00	3A4
ATOM	1943		SER	290 ·	45.026	1.325	33.179	1.00	0.00	3A4
ATOM	1944	OG	SER	290	43.728	1.835	32.895	1.00	0.00	3A4
MOTA	1945	С	SER	290	45.931	1.008	30.867	1.00	0.00	3A4
MOTA	1946	0	SER	290	45.432	1.483	29.847	1.00	0.00	3A4
MOTA	1947	N	ASP	291	46.293	-0.287	30.944	1.00	0.00	3A4
MOTA	1948	CA	ASP	291	46.226	-1.223	29.856	1.00	0.00	3A4
MOTA	1949	СВ	ASP	291	46.894	-2.555	30.218	1.00	0.00	3A4
ATOM	1950	CG	ASP	291	48.385	-2.331	30.513	1.00	0.00	3A4
ATOM ATOM	1951 1952	OD1 OD2		291 291	49.127 48.800	-1.982 -2.508	29.555 31.690	1.00	0.00	3A4 3A4
ATOM	1953	C	ASP	291	44.820	-1.495	29.390	1.00	0.00	3A4
ATOM	1954	ŏ	ASP	291	44.578	-1.735	28.227	1.00	0.00	3A4
ATOM	1955	N	LEU	292	43.831				0.00	3A4
ATOM	1956	CA	LEU	292	42.433	-1.624	29.999	1.00	0.00	3A4
ATOM	1957	СВ	LEU	292	41.659	-1.848	31.312	1.00	0.00	3A4
ATOM	1958	CG	LEU	292	41.910	-3.218	31.978	1.00	0.00	3A4
ATOM	1959	CD1		292	41.502	-3.197	33.463	1.00	0.00	3A4
ATOM	1960	CD2		292	41.193	-4.362	31.230	1.00	0.00	3A4
ATOM	1961	C	LEU	292	41.827	-0.445	29.268	1.00	0.00	3A4
ATOM	1962	0	LEU	292	41.078	-0.602	28.309	1.00	0.00	3A4
ATOM	1963	N	GLU	293	42.216	0.784	29.669	1.00	0.00	3A4 3A4
ATOM ATOM	1964 1965	CA CB	GLU GLU	293 293	41.794 42.258	2.025 3.233	29.064 29.892	1.00	0.00	3A4 3A4
ATOM	1966	CG	GLU	293	41.403	3.396	31.163	1.00	0.00	3A4
ATOM	1967	CD	GLU	293	41.950	4.520	32.046	1.00	0.00	3A4
ATOM	1968	OE1		293	41.285	4.842	33.067	1.00	0.00	3A4
ATOM	1969	OE2		293	43.037	5.066	31.722	1.00	0.00	3A4
ATOM	1970	C	GLU	293	42.286	2.186	27.666	1.00	0.00	3A4
ATOM	1971	0	GLU	293	41.540	2.607	26.793	1.00	0.00	· 3A4
MOTA	1972	N	LEU	294	43.547	1.769	27.420	1.00	0.00	3A4
ATOM	1973	CA	LEU	294	44.175	1.802	26.122	1.00	0.00	3A4

ATOM	1974	СВ	LEU	294	45.633	1.380	26.208	1.00	0.00	3A4
MOTA	1975	CG	LEU	294	46.091	-0.086	26.051	1.00	0.00	3A4
ATOM	1976		LEU	294 294 .	46.203 47.365	-0.637 -0.436	24.643 26.810	1.00	0.00	3A4 3A4
ATOM ATOM	1977 1978	CDZ	LEU	294	43.443	0.944	25.134	1.00	0.00	3A4
ATOM	1979	ŏ	LEU	294	43.172	1.361	24.020	1.00	0.00	3A4
MOTA	1980	N	VAL	295	43.044	-0.282	25.551	1.00	0.00	3A4
ATOM	1981	CA	VAL	295 295	42.358 42.271	-1.242 -2.600	24.721 25.380	1.00	0.00	3A4 3A4
ATOM ATOM	1982 1983	CB CG1	VAL VAL	295	41.397	-3.622	24.599	1.00	0.00	3A4
ATOM	1984		VAL	295	43.701	-3.178	25.429	1.00	0.00	3A4
ATOM	1985	С	VAL	295	40.980	-0.762	24.357	1.00	0.00	3A4
ATOM	1986	0	VAL ALA	295 296	40.584 40.252	-0.846 -0.146	23.207 25.306	1.00	0.00	3A4 3A4
ATOM ATOM	1987 1988	N CA	ALA	296	38.945	0.439	25.074	1.00	0.00	3A4
MOTA	1989	СВ	ALA	296	38.344	0.902	26.408	1.00	0.00	3A4
MOTA	1990	C	ALA	296	38.944	1.619	24.132	1.00	0.00	3A4
ATOM ATOM	1991 1992	O N	ALA GLN	296 297	38.032 40.018	1.797 2.430	23.342 24.170	1.00	0.00	3A4 3A4
ATOM	1993	CA	GLN	297	40.228	3.546	23.284	1.00	0.00	3A4
ATOM	1994	СВ	GLN	297	41.379	4.436	23.773	1.00	0.00	3A4
ATOM	1995	CG	GLN	297	40.914	5.233	25.008	1.00	0.00	3A4
ATOM .	1996 1997	CD OE1	GLN GLN	297 297	42.099 43.052	5.887 5.222	25.715 26.114	1.00	0.00	3A4 3A4
ATOM	1998	NE2	GLN	297	42.034	7.228	25.902	1.00	0.00	3A4
MOTA	1999	С	GLN	297	40.505	3.108	21.882	1.00	0.00	3A4
MOTA	2000	0	GLN	297	39.872	3.572	20.943	1.00	0.00	3A4 3A4
MOTA MOTA	2001 2002	N CA	SER SER	298 298	41.403	2.117 1.546	21.715 20.434	1.00	0.00	3A4
ATOM	2003	СВ	SER	298	42.925	0.563	20.529	1.00	0.00	3A4
ATOM	2004	OG	SER	298	42.771	-0.519	21.435	1.00	0.00	3A4
ATOM	2005	C	SER	298	40.584 40.435	0.872 0.977	19.755 18.546	1.00	0.00	3A4 3A4
ATOM ATOM	2006 2007	O N	SER ILE	298 299	39.688	0.228	20.542	1.00	0.00	3A4
ATOM	2008	CA	ILE	299	38.438	-0.363	20.098	1.00	0.00	3A4
ATOM	2009	СВ	ILE	299	37.670	-1.032	21.291	1.00	0.00	3A4
ATOM ATOM	2010 2011	CG2	ILE	299 · 299	36.134 38.328	-1.268 -2.333	21.098 21.803	1.00	0.00	3A4 3A4
ATOM	2012	CD	ILE	299	37.787	-3.619	21.185	1.00	0.00	3A4
MOTA	2013	C	ILE	299	37.515	0.677	19.534	1.00	0.00	3A4
ATOM	2014	0	ILE	299	36.949	0.525	18.457	1.00	0.00	3A4 3A4
ATOM ATOM	2015 2016	N CA	ILE	300 300	37.374 36.494	1.799	20.268 19.921	1.00	0.00	3A4
ATOM	2017	СВ	ILE	300	36.290	3.798	21.113	1.00	0.00	3A4
ATOM	2018	CG2	ILE	300	36.292	5.340	20.897	1.00		3A4
MOTA MOTA	2019 2020	CG1	ILE ILE	300 300	34.906 34.503	3.296 3.642	21.637 23.050	1.00	0.00	3A4 3A4
ATOM	2021	C	ILE	300	36.962	3.618	18.712	1.00	0.00	3A4
ATOM	2022	0	ILE	300	36.161	3.994	17.872	.1.00	0.00	3A4
ATOM	2023	N	PHE	301	38.279	3.774	18.515	1.00	0.00	3A4
ATOM ATOM	2024 2025	CA CB	PHE PHE	301 301	38.819 40.332	4.525 4.745	17.406 17.663	1.00	0.00	3A4 3A4
ATOM	2026	CG	PHE	301	40.520	5.958	18.535	1.00	0.00	3A4
ATOM	2027	CD1		301	41.157	5.931	19.784	1.00	0.00	3A4
ATOM	2028		PHE	301	39.913	7.144 7.015	18.106	1.00	0.00	3A4 3A4
MOTA MOTA	2029 2030		PHE PHE	301 301	41.032 39.784	8.213	20.660 18.969	1.00	0.00	3A4
ATOM	2031	cz	PHE	301	40.300	8.142	20.259	1.00	0.00	3A4
ATOM	2032	С	PHE	301	38.633	3.743	16.111	1.00	0.00	3A4
ATOM ATOM	2033 2034	O N	PHE	301 302	38.332 38.742	4.306 2.401	15.062 16.178	1.00	0.00	3A4 3A4
ATOM	2035	CA	ILE	302	38.511	1.491	15.076	1.00	0.00	3A4
MOTA	2036	СВ	ILE	302	39.005	0.104	15.470	1.00	0.00	3A4
MOTA	2037		ILE	302	38.482 40.563	-1.056	14.570	1.00	0.00	3A4 3A4
ATOM ATOM	2038 2039	CG1	ILE	302 302	40.563	0.105 0.195	15.527 14.178	1.00	0.00	3A4 3A4
ATOM	2040	c	ILE	302	37.054	1.462	14.656	1.00	0.00	3A4
MOTA	2041	0	ILE	302	36.732	1.682	13.491	1.00	0.00	3A4
ATOM ATOM	2042 2043	N CA	PHE PHE	303 303	36.126 34.711	1.231	15.610 15.324	1.00	0.00	3A4 3A4
ATOM	2043	CB	PHE	303	34.711	0.159	16.395	1.00	0.00	3A4
ATOM	2045	CG	PHE	303	33.072	0.735	17.449	1.00	0.00	3A4

ATOM	2046	CD1	PHE	303	31.783	1.209	17.127	1.00	0.00	3A4
ATOM	2047	CD2		303	33.443	0.706	18.808	1.00	0.00	3A4
ATOM	2048	CE1	PHE	303	30.911	1.674	18.121	1.00	0.00	3A4
MOTA	2049	CE2	PHE	303	32.572	1.155	19.810	1.00	0.00	3A4
ATOM	2050	CZ	PHE	303	31.307	1.647	19.465	1.00	0.00	3A4
MOTA	2051	С	PHE	303	34.016	2.407	14.993	1.00	0.00	3A4 3A4
MOTA	2052	0	PHE	303	33.183	2.472	14.092	1.00	0.00	3A4
ATOM	2053	N	ALA	304	34.391 33.814	3.513 4.831	15.679 15.484	1.00	0.00	3A4
ATOM	2054	CA	ALA	304 304	34.124	5.826	16.638	1.00	0.00	3A4
MOTA	2055 2056	CB C	ALA ALA	304	34.221	5.470	14.208	1.00	0.00	3A4
ATOM ATOM	2057	o	ALA	304	33.449	6.196	13.589	1.00	0.00	3A4
ATOM	2058	N	GLY	305	35.466	5.191	13.787	1.00	0.00	3A4
MOTA	2059	CA	GLY	305	36.037	5.755	12.599	1.00	0.00	3A4
ATOM	2060	C	GLY	305	35.766	5.044	11.304	1.00	0.00	3A4
MOTA	2061	0	GLY	305	36.028	5.603	10.243	1.00	0.00	3A4
MOTA	2062	N	TYR	306	35.257	3.789	11.337	1.00	0.00	3A4
ATOM	2063	CA	TYR	306	35.125	2.982	10.139	1.00	0.00	3A4
ATOM ·	2064	CB	TYR	306	35.531	1.484	10.389	1.00	0.00	3A4 3A4
ATOM	2065	CG	TYR	306	35.403	0.528 0.950	9.206 7.858	1.00	0.00	3A4
MOTA	2066		TYR	306 306	35.378 35.195	-0.835	9.469	1.00	0.00	3A4
ATOM	2067 2068		TYR TYR	306	35.009	0.064	6.843	1.00	0.00	3A4
ATOM ATOM	2069		TYR	306	34.885	-1.738	8.441	1.00	0.00	3A4
ATOM	2070	CZ	TYR	306	34.766	-1.281	7.125	1.00	0.00	3A4
ATOM	2071	ОН	TYR	306	34.383	-2.159	6.089	1.00	0.00	3A4
ATOM	2072	С	TYR	306	33.741	3.132	9.572	1.00	0.00	3A4
ATOM	2073	0	TYR	306	33.566	3.553	8.431	1.00	0.00	3A4
ATOM	2074	N	GLU	307	32.692	2.781	10.344	1.00	0.00	3A4
ATOM	2075	CA	GLU	307	31.384	2.639	9.745	1.00	0.00	3A4
ATOM	2076	CB	GLU	307	30.517	1.553	10.437	1.00	0.00	3A4 3A4
ATOM	2077	CG	GLU	307	31.119	0.127 -0.460	10.329 8.905	1.00	0.00	3A4
ATOM	2078	CD	GLU GLU	307 307	31.130 30.600	0.159	7.942	1.00	0.00	3A4
ATOM ATOM	2079 2080		GLU	307	31.670	-1.592	8.778	1.00	0.00	3A4
ATOM	2081	C	GLU	307	30.630	3.933	9.563	1.00	0.00	3A4
ATOM	2082	ŏ	GLU	307	29.605	3.926	8.924	1.00	0.00	3A4
ATOM	2083	N	THR	308	31.140	5.089	10.026	1.00	0.00	3A4
ΛΤΟM	2084	CA	THR	308	30.556	6.394	9.788	1.00	0.00	3A4
ATOM	2085	CB	THR	308	30.866	7.363	10.932	1.00	0.00	3A4
ATOM	2086		THR	308	32.255	7.423	11.254	1.00	0.00	3A4 3A4
ATOM	2087		THR	308	30.088	6.935 6.957	12.191 8.463	1.00	0.00	3A4
ATOM	2088	C	THR	308 308	31.006 30.202	7.360	7.632	1.00	0.00	3A4
ATOM	2089 2090	O N	THR THR	309	32.332		8.226	1.00	0.00	3A4
MOTA MOTA	2090	CA	THR	309	32.979	7.436	7.038	1.00	0.00	3A4
ATOM	2092	СВ	THR	309	34.479	7.445	7.204	1.00	0.00	3A4
ATOM	2093		THR	309	34.937	6.213	7.743	1.00	0.00	3A4
ATOM	2094	CG2	THR	309	34.867	8.555	8.200	1.00	0.00	3A.4
MOTA	2095	C	THR	309	32.600	6.684	5.779	1.00	0.00	3A4
ATOM	2096	0	THR	309	32.349	7.278	4.741	1.00	0.00	3A4 3A4
ATOM	2097	N	SER	310	32.484	5.339	5.875 4.809	1.00	0.00	3A4
ATOM	2098	CA CB	SER SER	310 310	32.052 31.996	4.458 2.990	5.310	1.00	0.00	3A4
ATOM	2099 2100	OG	SER	310	33.306	2.563	5.646	1.00	0.00	3A4
MOTA MOTA	2101	c	SER	310	30.666	4.763	4.322	1.00	0.00	3A4
ATOM	2102	ŏ	SER	310	30.413	4.886	3.131	1.00	0.00	3A4
ATOM	2103	N	SER	311	29.728	4.960	5.261	1.00	0.00	3A4
ATOM	2104	CA	SER	311	28.351	5.245	4.950	1.00	0.00	3A4
ATOM	2105	CB	SER	311	27.509	5.056	6.222	1.00	0.00	3A4
MOTA	2106	OG	SER	311	27.701	3.739	6.719	1.00	0.00	3A4
ATOM	2107	C	SER	311	28.153	6.627	4.389	1.00	0.00	3A4 3A4
ATOM	2108	0	SER	311	27.316	6.833 7.609	3.523 4.813	1.00	0.00	3A4
ATOM	2109	N	VAL	312	28.984 28.964	8.970	4.813	1.00	0.00	3A4
ATOM	2110 2111	CA CB	VAL VAL	312 312	29.781	9.902	5.173	1.00	0.00	3A4
MOTA MOTA	2111		VAL	312	29.980	11.315	4.570	1.00	0.00	3A4
ATOM	2113		VAL	312	28.894	10.077	6.433	1.00	0.00	3A4
ATOM	2114	c	VAL	312	29.408	9.072	2.884	1.00	0.00	3A4
ATOM	2115	ō	VAL	312	28.751	9.739	2.103	1.00	0.00	3A4
MOTA	2116	N	LEU	313	30.463	8.328	2.495	1.00	0.00	3A4
ATOM	2117	CA	LEŲ	313	30.996	8.277	1.150	1.00	0.00	3A4

ATOM	2118	СВ	LEU	313	32.294	7.466	1.085	1.00	0.00	3A4
MOTA	2119	CG	LEU	313	33.512	8.219	1.649	1.00	0.00	3A4
ATOM	2120	CD1	LEU	313	34.492	8.511	0.499	1.00	0.00	3A4
MOTA	2121		LEU	313	33.322	9.485	2.496	1.00	0.00	3A4
ATOM	2122	C	LEU	313	30.017	7.696	0.167	1.00	0.00	3A4
MOTA	2123	0	LEU	313	29.808	8.229	-0.917	1.00	0.00	3A4 3A4
MOTA	2124	N	SER	314	29.309	6.624	0.579 -0.243	1.00	0.00	3A4
ATOM	2125	CA	SER	314	28.305 27.992	5.981 4.570	0.299	1.00	0.00	3A4
ATOM	2126	CB OG	SER SER	314 314	29.195	3.821	0.397	1.00	0.00	3A4
MOTA MOTA	2127 2128	C	SER	314	27.070	6.845	-0.420	1.00	0.00	3A4
ATOM	2129	ō	SER	314	26.505	6.909	-1.507	1.00	0.00	3A4
ATOM	2130	N	PHE	315	26.702	7.636	0.625	1.00	0.00	3A4
ATOM	2131	CA	PHE	315	25.595	8.572	0.583	1.00	0.00	3A4
ATOM	2132	СВ	PHE	315	25.181	9.076	2.015	1.00	0.00	3A4
MOTA	2133	CG	PHE	315	23.897	8.407	2.456	1.00	0.00	3A4
ATOM	2134		PHE	315	23.856	7.678	3.662	1.00	0.00	3A4
ATOM	2135		PHE	315	22.732	8.451	1.660	1.00	0.00	3A4
ATOM	2136		PHE	315	22.683	7.024	4.067	1.00	0.00	3A4 3A4
ATOM	2137		PHE	315	21.568 21.542	7.770 7.061	2.047 3.254	1.00	0.00	3A4
ATOM	2138	CZ	PHE PHE	315 315	25.938	9.760	-0.291	1.00	0.00	3A4
ATOM ATOM	2139 2140	С 0	PHE	315	25.075	10.250	-1.011	1.00	0.00	3A4
ATOM	2141	N	ILE	316	27.230	10.200	-0.328	1.00	0.00	3A4
ATOM	2142	CA	ILE	316	27.669	11.286	-1.202	1.00	0.00	3A4
ATOM	2143	СВ	ILE	316	29.119	11.864	-1.060	1.00	0.00	3A4
ATOM	2144		ILE	316	29.128	13.291	-1.688	1.00	0.00	3A4
MOTA	2145	CG1	ILE	316	29.687	11.833	0.371	1.00	0.00	3A4
MOTA	2146	CD	ILE	316	30.950	12.629	0.687	1.00	0.00	3A4
MOTA	2147	С	ILE	316	27.559	10.926	-2.666	1.00	0.00	3A4 3A4
ATOM	2148	0	ILE	316	27.111	11.726	-3.476 -3.009	1.00	0.00	3A4
ATOM	2149	N	MET	317 317	27.919 27.868	9.671 9.137	-4.351	1.00	0.00	3A4
ATOM ATOM	2150 2151	CA CB	MET MET	317	28.640	7.803	-4.441	1.00	0.00	3A4
ATOM	2152	CG	MET	317	30.148	8.007	-4.191	1.00	0.00	3A4
ATOM	2153	SD	MET	317	31.027	6.548	-3.550	1.00	0.00	3A4
ATOM	2154	CE	MET	317	32.475	7.489	-2.987	1.00	0.00	3A4
ATOM	2155	С	MET	317	26.449	8.978	-4.853	1.00	0.00	3A4
MOTA	2156	0	MET	317	26.139	9.327	-5.986	1.00	0.00	3A4
MOTA	2157	N	TYR	318	25.516	8.539	-3.981	1.00	0.00	3A4
ATOM	2158	CA	TYR	318	24.101	8.458	-4.293	1.00	0.00	3A4 3A4
MOTA	2159	CB	TYR	318	23.333	7.794	-3.134 -3.312	1.00	0.00	3A4
	2160	CG	TYR	318	21.822 21.269	7.683 7.039	-4.436	1.00	0.00	3A4
ATOM	2161 2162		TYR TYR	318 318	. 20.950	8.269	-2.372	1.00	0.00	3A4
ATOM ATOM	2163		TYR	318	19.881	6.987	-4.624	1.00	0.00	3A4
ATOM	21.64		TYR	318	19.560	8.209	-2.548	1.00	0.00	3A4
ATOM	2165	cz	TYR	318	19.024	7.566	-3.675	1.00	0.00	3A4
ATOM	2166	ОН	TYR	318	17.625	.7.498	-3.855	1.00	0.00	. 3A4
MOTA	2167	C	TYR	318	23.501	9.814	-4.592	1.00	0.00	3A4
MOTA	2168	0	TYR	318	22.759	9.967	-5.553	1.00	0.00	3A4
MOTA	2169	И	GLU	319	23.864	10.847	-3.796	1.00	0.00	3A4 3A4
MOTA	2170	CA	GLU	319	23.389	12.203 13.127	-3.970 -2.775	1.00	0.00	3A4
MOTA	2171	CB	GLU	319	22.849	12.760	-1.559	1.00	0.00	3A4
MOTA MOTA	2172 2173	CG CD	GTN GTN	319 319	23.038	13.838	-0.506	1.00	0.00	3A4
ATOM	2174		GLU	319	24.202	14.049	-0.085	1.00	0.00	3A4
ATOM	2175		GLU	319	22.027	14.476	-0.119	1.00	0.00	3A4
ATOM	2176	c	GLU	319	23.894	12.847	-5.231	1.00	0.00	3A4
MOTA	2177	0	GLU	319	23.132	13.474	-5.951	1.00	0.00	3A4
MOTA	2178	N	LEU	320	25.170	12.641	-5.595	1.00	0.00	3A4
ATOM	2179	CA	LEU	320	25.713	13.161	-6.828	1.00	0.00	3A4
MOTA	2180	СВ	LEU	320	27.239	13.059	-6.841	1.00	0.00	3A4
ATOM	2181	CG	LEU	320	27.880	14.027	-5.843	1.00	0.00	3A4 3A4
ATOM	2182		LEU	320	29.380	13.757	-5.709 -6.192	1.00	0.00	3A4
ATOM	2183		LEU	320 320	27.611 25.160	15.489 12.475	-8.048	1.00	0.00	3A4
MOTA MOTA	2184 2185	С 0	LEU LEU	320	24.977	13.105	-9.083	1.00	0.00	3A4
ATOM	2186	N	ALA	321	24.818	11.177	-7.933	1.00	0.00	3A4
ATOM	2187	CA	ALA	321	24.215	10.397	-8.990	1.00	0.00	3A4
ATOM	2188	СВ	ALA	321	24.217	8.897	-8.645	1.00	0.00	3A4
ATOM	2189	C	ALA	321	22.802	10.861	-9.259	1.00	0.00	3A4

ATOM	2190	0	ALA	321	22.338	10.884	-10.397	1.00	0.00	3A4
ATOM	2191	N	THR	322	22.103	11.305	-8.194	1.00	0.00	3A4
ATOM	2192	CA	THR	322	20.743	11.780	-8.258	1.00	0.00	3A4
ATOM	2193	СВ	THR	322	19.981	11.519	-6.972	1.00	0.00	3A4
ATOM	2194	0G1	THR	322	20.610	11.999	-5.794	1.00	0.00	3A4
ATOM	2195	CG2		322	19.745	9.994	-6.849	1.00	0.00	3A4
ATOM	2196	С	THR	322	20.627	13.242	-8.642	1.00	0.00	3A4
ATOM	2197	0	THR	322	19.555	13.704	-9.018	1.00	0.00	3A4
MOTA	2198	N	HIS	323	21.731	14.006	-8.558	1.00	0.00	3A4
ATOM	2199	CA	HIS	323	21.740	15.416	-8.856	1.00	0.00	3A4
MOTA	2200	ND1	HIS	323	20.544	15.212	-5.650	1.00	0.00	3A4
ATOM	2201	CG	HIS	323	20.676	16.147	-6.653	1.00	0.00	3A4
ATOM	2202	СВ	HIS	323	21.859	16.259	-7.581	1.00	0.00	3A4
ATOM	2203	NE2	HIS	323	18.715	16.470	-5.582	1.00	0.00	3A4
ATOM	2204	CD2	HIS	323	19.549	16.908	-6.595	1.00	0.00	3A4
MOTA	2205	CE1		323	19.356	15.449	-5.043	1.00	0.00	3A4
ATOM	2206	С	HIS	323	22.892	15.711	-9.775	1.00	0.00	3A4
ATOM	2207	0	HIS	323	23.883	16.309	-9.352	1.00	0.00	3A4
ATOM	2208	N	PRO	324	22.833		-11.076	1.00	0.00	3A4 3A4
MOTA	2209	CA	PRO	324	23.958		-12.002	1.00	0.00	3A4
ATOM	2210	CD	PRO	324	21.602		-11.765	1.00	0.00	3A4
MOTA	2211	CB	PRO	324	23.420		-13.300	1.00	0.00	3A4
MOTA	2212	CG	PRO	324	21.905		-13.255	1.00	0.00	3A4
ATOM	2213	С	PRO	324	24.415		-12.213	1.00	0.00	3A4
MOTA	2214	0	PRO	324	25.575		-12.534	1.00	0.00	3A4
ATOM	2215	N	ASP	325	23.561		-11.949	1.00	0.00	3A4
ATOM	2216	CA	ASP	325	23.917		-12.002	1.00	0.00	3A4
ATOM	2217	CB	ASP	325	22.668 21.653		-11.821 -12.931	1.00	0.00	3A4
ATOM	2218	CG	ASP	325	21.833		-14.125	1.00	0.00	3A4
ATOM	2219		ASP	325	20.531		-12.600	1.00	0.00	3A4
ATOM	2220		ASP ASP	325 325	24.927		-10.944	1.00	0.00	3A4
ATOM	2221 2222	C O	ASP	325	25.817		-11.169	1.00	0.00	3A4
ATOM ATOM	2223	N	VAL	326	24.835	19.071	-9.767	1.00	0.00	3A4
ATOM	2224	CA	VAL	326	25.742	19.249	-8.647	1.00	0.00	3A4
ATOM	2225	·CB	VAL	326	25.198	18.672	-7.341	1.00	0.00	3A4
ATOM	2226		VAL	326	26.201	18.872	-6.173	1.00	0.00	3A4
ATOM	2227		VAL	326	23.874	19.402	-7.034	1.00	0.00	3A4
ATOM	2228	c	VAL	326	27.083	18.648	-8.960	1.00	0.00	3A4
ATOM	2229	ō	VAL	326	28.106	19.288	-8.782	1.00	0.00	3A4
ATOM	2230	N	GLN	327	27.089	17.427	-9.528	1.00	0.00	3A4
ATOM	2231	CA	GLN	327	28.281	16.718	-9.931	1.00	0.00	3A4
ATOM	2232	СВ	GLN	327	27.899		-10.487	1.00	0.00	3A4
MOTA	2233	CG	GLN	327	29.062		-10.683	1.00	0.00	3A4
ATOM	2234	CD	GLN	327	28.538		-11.166	1.00	0.00	3A4
ATOM	2235	OE1	GLN	327	27.336		-11.186	1.00	0.00	3A4
MOTA	2236	NE2	GLN	327	29.475		-11.572	1.00	0.00	3A4
ATOM	2237	С	GLN	327	29.088		-10.960	1.00	0.00	3A4
ATOM	2238	0	GLN	327	30.301	_	-10.855	1.00	0.00	3A4
ATOM	2239	N	GLN	328	28.408		-11.941	1.00	0.00	3A4 3A4
ATOM	2240	CA	GLN	328	29.023		-12.995	1.00	0.00	3A4
ATOM	2241	CB	GLN	328	27.977		-14.041	1.00	0.00	3A4
ATOM	2242	CG	GLN	328	27.544		-14.957 -15.885	1.00	0.00	3A4
MOTA	2243	CD	GLN	328	26.423		-16.800	1.00	0.00	3A4
ATOM	2244		GLN	328	26.675		-15.654	1.00	0.00	3A4
MOTA	2245		GLN	328 328	25.164 29.711		-12.470	1.00	0.00	3A4
MOTA	2246	C	GLN	328	30.827		-12.855	1.00	0.00	3A4
ATOM ATOM	2247 2248	0	GLN	329	29.068		-11.501	1.00	0.00	3A4
	2249	N CA	LYS LYS	329	29.597		-10.807	1.00	0.00	3A4
ATOM ATOM	2250	СВ	LYS	329	28.515	22.465		1.00	0.00	3A4
ATOM	2251	CG	LYS	329	28.752	23.857		1.00	0.00	3A4
ATOM	2252	CD	LYS	329	27.533	24.347		1.00	0.00	3A4
ATOM	2253	CE	LYS	329	27.679	25.785	_	1.00	0.00	3A4
ATOM	2254	NZ	LYS	329	26.477	26.210		1.00	0.00	3A4
ATOM	2255	c	LYS	329	30.884		-10.052	1.00	0.00	3A4
ATOM	2256	ō	LYS	329	31.860	22.366	-10.101	1.00	0.00	3A4
ATOM	2257	N	LEU	330	30.952	20.423	-9.426	1.00	0.00	3A4
MOTA	2258	CA	LEU	330	32.100	19.968	-8.670	1.00	0.00	3A4
ATOM	2259	СВ	LEU	330	31.814	18.742			0.00	3A4
MOTA	2260	CG	LEU	330	30.502	18.756			0.00	3A4
ATOM	2261		LEU	330	30.541	17.732	-5.920	1.00	0.00	3A4

MOTA	2262	CD2	LED	330	29.986	20.145 -6.584	1.00	0.00	3A4
ATOM	2263	c	LEU	330	33.250	19.598 -9.579	1.00	0.00	3A4
ATOM	2264	Ö	LEU	330	34.410	19.864 -9.296	1.00	0.00	3A4
			GLN	331	32.931	18.993 -10.741	1.00	0.00	3A4
ATOM	2265	N.		331	33.881	18.627 -11.762	1.00	0.00	3A4
MOTA	2266	CA	GLN		33.229	17.787 -12.880	1.00	0.00	3A4
MOTA	2267	CB	GLN	331		16.354 -12.389	1.00	0.00	3A4
ATOM	2268	CG	GLN	331	32.942		1.00	0.00	3A4
MOTA	2269	CD	GLN	331	32.147	15.568 -13.437		0.00	3A4
MOTA	2270	OE1		331	31.063	15.988 -13.839	1.00		
MOTA	2271	NE2		331	32.677	14.396 -13.885	1.00	0.00	3A4
ATOM	2272	С	GLN	331	34.500	19.817 -12.447	1.00	0.00	3A4
MOTA	2273	0	GLN	331	35.682	19.821 -12.771	1.00	0.00	3A4
MOTA	2274	N	GLU	332	33.723	20.913 -12.594	1.00	0.00	3A4
ATOM	2275	CA	GLU	332	34.188	22.185 -13.099	1.00	0.00	3A4
ATOM	2276	CB	GLU	332	33.019	23.173 -13.413	1.00	0.00	3A4
ATOM	2277	CG	GLU	332	32.212	22.808 -14.675	1.00	0.00	3A4
ATOM	2278	CD	GLU	332	33.080	22.951 -15.931	1.00	0.00	3A4
ATOM	2279	OE1	GLU	332	33.533	24.092 -16.217	1.00	0.00	3A4
ATOM	2280	OE2	GLU	332	33.301	21.919 -16.622	1.00	0.00	3A4
ATOM	2281	С	GLU	332	35.190	22.869 -12.182	1.00	0.00	3A4
ATOM	2282	o	GLU	332	35.834	23.799 -12.629	1.00	0.00	3A4
ATOM	2283	N	GLU	333	35.484	22.350 -10.947	1.00	0.00	3A4
ATOM	2284	CA	GLU	333	36.662	22.661 -10.132	1.00	0.00	3A4
ATOM	2285	СВ	GLU	333	36.449	22.284 -8.639	1.00	0.00	3A4
ATOM .	2286	CG	GLU	333	35.228	22.936 -7.985	1.00	0.00	3A4
ATOM	2287	CD	GLU	333	35.046	22.273 -6.620	1.00	0.00	3A4
		OE1		333	35.918	22.455 -5.730	1.00	0.00	3A4
ATOM	2288	OE2			34.038	21.540 -6.462	1.00	0.00	3A4
ATOM	2289			333	37.923	21.912 -10.581	1.00	0.00	3A4
ATOM	2290	C	GLU	333		21.038 -9.874	1.00	0.00	3A4
ATOM	2291	0	GLU	333	38.425	22.262 -11.773	1.00	0.00	3A4
ATOM	2292	N	ILE	334	38.469			0.00	3A4
ATOM	2293	CA	ILE	334	39.710	21.726 -12.300	1.00		3A4
MOTA	2294	СВ	ILE	334	39.559	20.353 -12.973	1.00	0.00	3A4
ATOM	2295	CG2	ILE	334	38.582	20.368 -14.182	1.00	0.00	
ATOM	2296	CG1	ILE	334	40.932	19.687 -13.257	1.00	0.00	3A4
ATOM	2297	CD	ILE	334	40.838	18.213 -13.660	1.00	0.00	3A4
ATOM	2298	С	ILE	334	40.231	22.836 -13.189	1.00	0.00	3A4
ATOM	2299	0	ILE	334	40.570	22.658 -14.358	1.00	0.00	. 3A4
ATOM	2300	N	ASP	335	40.294	24.063 -12.600	1.00	0.00	3A4
ATOM	2301	CA	ASP	335	40.593	25.320 -13.260	1.00	0.00	3A4
ATOM	2302	CB	ASP	335	39.726	26.490 -12.699	1.00	0.00	3A4
ATOM	2303	CG	ASP	335	38.240	26.203 -12.943	1.00	0.00	3A4
ATOM	2304	OD1	ASP	335	37.854	26.015 -14.129	1.00	0.00	3A4
ATOM	2305	OD2	ASP	335	37.469	26.175 -11.947	1.00	0.00	3A4
ATOM	2306	С	ASP	335	42.054	25.655 -13.079	1.00	0.00	3A4
ATOM	2307	0	ASP	335	42.537	25.781 -11.956	1.00	0.00	3A4
ATOM	2308	N	ALA	336	42.772	25.816 -14.223	1.00	0.00	3A4
ATOM	2309	CA	ALA	336	44.168	26.192 -14.316	1.00	0.00	3A4
ATOM	2310	СB	ALA	336	45.027	25.116 -15.028	1.00	0.00	3A4
ATOM	2311	c	ALA	336	44.207	27.500 -15.065	1.00	0.00	3A4
ATOM	2312	ŏ	ALA	336	44.428	27.544 -16.275	1.00	0.00	. 3A4
ATOM	2312	N	VAL	337	43.963	28.609 -14.313	1.00	0.00	3A4
ATOM	2314	CA	VAL	337	43.815	29.978 -14.773	1.00	0.00	3A4
	2315	СВ	VAL	337	42.641	30.686 -14.085	1.00	0.00	3A4
ATOM ATOM	2316		VAL	337	42.436	32.130 -14.612	1.00	0.00	3A4
			VAL	337	41.367	29.847 -14.326	1.00	0.00	3A4
ATOM	2317			337	45.115	30.696 -14.492	1.00	0.00	3A4
ATOM	2318	C	VAL		45.661	30.605 -13.394	1.00	0.00	3A4
ATOM	2319	0	VAL	337		31.439 -15.517	1.00	0.00	3A4
ATOM	2320	N	LEU	338	45.621		1.00	0.00	3A4
ATOM	2321	CA	LEU	338	46.821	32.257 -15.500		0.00	3A4
ATOM	2322	СВ	LEU	338	47.678	32.088 -16.799	1.00	0.00	3A4
ATOM	2323	CG	LEU	338	48.507	30.778 -16.897	1.00		3A4
MOTA	2324		LEU	338	47.680	29.494 -17.124	1.00	0.00	· 3A4
ATOM	2325		LEU	338	49.592	30.909 -17.984	1.00	0.00	
MOTA	2326	С	LEU	338	46.355	33.705 -15.361	1.00	0.00	3A4
MOTA	2327	0	LEU	338	45.265	34.009 -15.844	1.00	0.00	3A4
MOTA	2328	N	PRO	339	47.103	34.638 -14.719	1.00	0.00	3A4
MOTA	2329	CA	PRO	339	46.612	35.949 -14.286	1.00	0.00	3A4
MOTA	2330	CD	PRO	339	48.443	34.363 -14.196	1.00	0.00	3A4
MOTA	2331	CB	PRO	339	47.610	36.376 -13.189	1.00	0.00	3A4
MOTA	2332	CG	PRO	339	48.922	35.669 ~13.552	1.00	0.00	3A4
ATOM	2333	С	PRO	339	46.561	36.955 -15.437	1.00	0.00	3A4

MOTA	2334	0	PRO	339	47.465	36.980	-16.272	1.00	0.00	3A4
ATOM	2335	N	ASN	340	45.491		-15.465	1.00	0.00	3A4
MOTA	2336	CA	ASN	340	45.246	38.810		1.00	0.00	3A4 3A4
MOTA	2337	СВ	ASN	340	44.189		-17.523	1.00	0.00	3A4
ATOM	2338	CG OD1	ASN	340 340	44.036 42.986		-18.704 -18.858	1.00	0.00	3A4
MOTA MOTA	2339 2340	ND2		340	45.094		-19.550	1.00	0.00	3A4
ATOM	2341	C	ASN	340	44.785		-15.672	1.00	0.00	3A4
ATOM	2342	ō ·	ASN	340	45.452		-15.645	1.00	0.00	3A4
ATOM	2343	N	LYS	341	43.617		-14.997	1.00	0.00	3A4 3A4
ATOM	2344	CA	LYS	341	43.059 42.250		-14.095 -14.822	1.00	0.00	3A4
ATOM ATOM	2345 2346	CB CG	LYS	341 341	41.892		-13.936	1.00	0.00	3A4
ATOM	2347	CD	LYS	341	41.220		-14.664	1.00	0.00	3A4
ATOM	2348	CE	LYS	341	39.708		-14.924	1.00	0.00	3A4
MOTA	2349	NZ	LYS	341	39.409		-15.994	1.00	0.00	3A4 3A4
ATOM	2350	C	LYS	341	42.197 40.991		-13.158 -13.036	1.00 1.00	0.00 0.00	3A4
ATOM ATOM	2351 2352	N N	LYS ALA	341 342	42.834		-12.482	1.00	0.00	3A4
ATOM	2353	CA	ALA	342	42.189		-11.577	1.00	0.00	3A4
ATOM	2354	СВ	ALA	342	41.316	37.064	-12.306	1.00	0.00	3A4
ATOM	2355	С	ALA	342	43.313		-10.839	1.00	0.00	3A4 3A4
ATOM	2356	0	ALA	342	44.413 43.106	36.880	-11.386 -9.614	1.00 1.00	0.00	3A4
MOT'A MOT'A	2357 2358	N CA	PRO PRO	343 343	44.072	36.050	-8.891	1.00	0.00	3A4
ATOM	2359	CD	PRO	343	41.953	37.220	-8.779	1.00	0.00	3A4
ATOM	2360	СВ	PRO		43.605	36.121	-7.421	1.00	0.00	3A4
ATOM	2361	CG	PRO	343	42.097	36.392	-7.496	1.00	0.00	3A4
ATOM	2362	C	PRO	343	44.071	34.607	-9.441 -9.619	1.00	0.00	3A4 3A4
ATOM. ATOM	2363 2364	N N	PRO PRO	343 344	42.970 45.209	34.083 33.930	-9.727	1.00	0.00	3A4
ATOM	2365	CA	PRO	344	45.259		-10.448	1.00	0.00	3A4
ATOM	2366	CD	PRO	344	- 46.542	34.509	-9.559	1.00	0.00	3A4
MOTA	2367	CB	PRO	344	46.678		-11.047	1.00	0.00	3A4 3A4
MOTA	2368	CG	PRO	344	47.532	33.459	-10.077 -9.520	1.00	0.00	3A4
ATOM ATOM	2369 2370	0	PRO PRO	344 344	45.002 45.522	31.443	-8.404	1.00	0.00	3A4
ATOM	2371	N	THR	345	44.206		-10.004	1.00	0.00	3A4
ATOM	2372	CA	THR	345	43.860	29.247	-9.324	1.00	0.00	3A4
ATOM	2373	CB	THR	345	42.343	29.124	-9.107	1.00	0.00 0.00	3A4 3A4
ATOM	2374 2375		THR THR	345 345	41.981 41.532	27.994	-8.315 -10.430	1.00	0.00	3A4
ATOM ATOM	2376	C	THR	345	44.457		-10.173	1.00	0.00	3A4
ATOM	2377	ō	THR	345	44.489	28.242	-11.397	1.00	0.00	3A4
ATOM	2378	N	TYR	346	44.964	27.063	-9.521	1.00	0.00	3A4 3A4
MOTA	2379	CA	TYR	346	45.601		-10.173 -10.121	1.00	0.00	3A4
ATOM ATOM	2380 2381	CB CG	TYR TYR	346 346	47.162 47.679		-10.925	1.00	0.00	3A4
ATOM	2382		TYR	346	48.250		-10.287	1.00	0.00	3A4
ATOM	2383		TYR	346	47.581		-12.331	1.00	0.00	3A4
MOTA	2384		TYR	346	48.713		-11.032	1.00	0.00	3A4 3A4
MOTA	2385		TYR	346	48.037 48.606		-13.082 -12.431	1.00	0.00	3A4
ATOM ATOM	2386 2387	CZ OH	TYR TYR	346 346	49.065		-13.178	1.00	0.00	3A4-
ATOM	2388	c	TYR	346	45.106	24.709		1.00	0.00	3A4
MOTA	2389	٥	TYR	346	45.423	24.491		1.00	0.00	3A4
MOTA	2390	N	ASP	347	44.302		-10.168 -9.683	1.00	0.00	3A4 3A4
ATOM ATOM	2391 2392	CA CB	ASP ASP	347 347	43.715 42.187	22.647 22.761		1.00	0.00	3A4
ATOM	2392	CG	ASP	347	41.948	23.760		1.00	0.00	3A4
ATOM	2394		ASP	347	41.329	24.825		1.00	0.00	3A4
ATOM	2395		ASP	347	42.386	23.474		1.00	0.00	3A4 3A4
ATOM	2396	C	ASP	347 347	43.937 43.549		-10.781 -11.927	1.00	0.00	3A4
ATOM ATOM	2397 2398	о И	ASP THR	347 348	44.581		-10.427	1.00	0.00	3A4
ATOM	2399	CA	THR	348	44.908	19.388	-11.314	1.00	0.00	3A4
ATOM	2400	CB	THR	348	46.416		-11.501	1.00	0.00	3A4
ATOM	2401		THR	348	46.987		-12.006	1.00	0.00	3A4 3A4
ATOM	2402 2403		THR	348 348	46.725 44.258		-12.500 -10.688	1.00	0.00	3A4
ATOM ATOM	2403	c o	THR	348	43.393		-11.293	1.00	0.00	3A4
ATOM	2405	N	VAL	349	44.670	17.854		1.00	0.00	3A4

MOTA	2406	CA	VAL	349	44.059	16.848	-8.590	1.00	0.00		3A4
ATOM	2407	CB	VAL '	349	44.630	15.437	-8.788	1.00	0.00		3A4
MOTA	2408		VAL	349	46.169	15.347	-8.617	1.00	0.00		3A4
ATOM	2409		VAL	349	43.834	14.402	-7.958	1.00	0.00		3A4
MOTA	2410	C	VAL	349	44.175	17.435	-7.201	1.00	0.00		3A4 3A4
ATOM	2411	0	VAL	349	44.934	16.990	-6.341	1.00	0.00		3A4
MOTA	2412	N	LEU	350	43.387 43.440	18.518 19.369	-6.988 -5.824	1.00	0.00		3A4
MOTA MOTA	2413 2414	CA CB	LEU	350 350	44.479	20.520	-6.024	1.00	0.00	·	3A4
ATOM	2415	CG	LEU	350	44.847	21.374	-4.785	1.00	0.00		3A4
ATOM	2416		LEU	350	45.497	20.539	-3.662	1.00	0.00		3A4
MOTA	2417		LEU	350	45.743	22.560	-5.187	1.00	0.00		3A4
ATOM	2418	С	LEU	350	42.042	19.913	-5.672	1.00	0.00		3A4
ATOM	2419	0	LEU	350	41.270	19.945	-6.631	1.00	0.00		3A4
MOTA	2420		.GLN	351	41.689	20.372	-4.436	1.00	0.00		3A4
ATOM	2421	CA	GLN	351	40.404	20.942	-4.059	1.00	0.00		3A4
MOTA	2422	CB	GLN	351	40.005	20.645	-2.573	1.00	0.00		3A4 3A4
MOTA	2423	CG	GLN	351	40.814 42.269	21.289 20.816	-1.417 -1.386	1.00	0.00		3A4
ATOM ATOM	2424 2425	CD	GLN GLN	351 351	42.209	21.634	-1.520	1.00	0.00		3A4
ATOM	2426		GLN	351	42.505	19.487	-1.200	1.00	0.00		3A4
ATOM	2427	c	GLN	351	40.390	22.432	-4.305	1.00	0.00		3A4
ATOM	2428	ō	GLN	351	41.399	23.112	-4.117	1.00	0.00		3A4
ATOM	2429	N	MET	352	39.214	22.962	-4.740	1.00	0.00		3A4
MOTA	2430	CA	MET	352	38.994	24.368	-5.014	1.00	0.00		3A4
ATOM	2431	CB	MET	352	38.436	24.632	-6.438	1.00	0.00		3A4
MOTA	2432	CG	MET	352	38.472	26.097	-6.900	1.00	0.00		3A4
ATOM	2433	SD	MET	352	37.969	26.316	-8.633 -8.608	1.00	0.00		3A4 3A4
ATOM	2434	CE	MET	352 352	38.075 38.113	28.129 24.911	-3.914	1.00	0.00		3A4
MOTA MOTA	2435 2436	С 0	MET MET	352	38.636	25.287	-2.866	1.00	0.00		3A4
ATOM	2437	N	GLU	353	36.765	25.000	-4.117	1.00	0.00		3A4
ATOM	2438	CA	GLU	353	35.914	25.749	-3.211	1.00	0.00		3A4
ATOM	2439	CB	GLU	353	35.689	27.217	-3.688	1.00	0.00		3A4
ATOM	2440	CG	GLU	353	36.922	28.142	-3.627	1.00	0.00		3A4
ATOM	2441	CD	GLU	353	36.543	29.540	-4.126	1.00	0.00		3A4
ATOM	2442		GLU	353	36.622	30.504	-3.318	1.00	0.00		3A4
ATOM	2443		GLU	353	36.171	29.660	-5.325	1.00	0.00		3A4 3A4
ATOM ATOM	2444 2445	С 0	GLU GLU	353 353	34.592 34.078	25.102 25.104	-2.984 -1.864	1.00	0.00		3A4
ATOM	2446	N	TYR	354	33.979	24.537	-4.047		0.00		3A4
MOTA	2447	CA	TYR	354	32.629	24.016	-3.996	1.00	0.00		3A4
ATOM	2448	СВ	TYR	354	31.928	24.005	-5.369	1.00	0.00		3A4
ATOM	2449	CG	TYR	354	31.880	25.395	-5.954	1.00	0.00		3A4
MOTA	2450	CD1	TYR	354	32.962	25.916	-6.691	1.00	0.00		3A4
ATOM	2451		TYR	354	30.740	26.199	-5.783	1.00	0.00		3A4
ATOM	2452		TYR	354	32.917	27.212	-7.224	1.00	0.00		3A4
ATOM	2453		TYR	354	30.683	27.496	-6.314 -7.035	1.00	0.00		3A4 3A4
ATOM ATOM	2454. 2455	CZ OH	TYR TYR	354 354	31.774 31.722	28.004 29.310	-7.571	1.00	0.00	•	3A4
ATOM	2456	C	TYR	354	32.592	22.628	-3.428	1.00	0.00		3A4
ATOM	2457	ŏ	TYR	354	31.575	22.220	-2.892	1.00	0.00		3A4
ATOM	2458	N	LEU	355	33.710	21.867	-3.466	1.00	0.00		3A4
MOTA	2459	CA	LEU	355	33.715	20.493	-2.996	1.00	0.00		3A4
MOTA	2460	CB	LEU	355	34.970	19.771	-3.512	1.00	0.00		3A4
MOTA	2461	CG	LEU	355	34.521	18.784	-4.631	1.00	0.00		3A4
ATOM	2462		LEU	355	35.547	18.525	-5.749	1.00	0.00		3A4
ATOM	2463		LEU	355	33.945	17.479	-4.064	1.00	0.00		3A4 3A4
ATOM	2464 2465	C	LEU	355 355	33.573 32.806	20.380 19.570	-1.485 -0.980	1.00	0.00		3A4
MOTA MOTA	2465	O N	LEU ASP	356	34.225	21.283	-0.721	1.00	0.00		3A4
ATOM	2467	CA	ASP	356	34.070	21.466	0.714	1.00	0.00		3A4
ATOM	2468	СВ	ASP	356	34.921	22.723	1.144	1.00	0.00		3A4
ATOM	2469	CG	ASP	356	35.819	22.461	2.358	1.00	0.00		3A4
ATOM	2470		ASP	356	35.262	22.182	3.454	1.00	0.00		3A4
ATOM	2471		ASP	356	37.067	22.560	2.214	1.00	0.00		3A4
ATOM	2472	C	ASP	356	32.651	21.700	1.182	1.00	0.00		3A4
ATOM	2473	0	ASP	356	32.180	21.110	2.149	1.00	0.00		3A4 3A4
MOTA MOTA	2474 2475	N CA	MET MET	357 357	31.928 30.540	22.551 22.879	0.423 0.616	1.00	0.00		3A4
ATOM	2476	CB	MET	357	30.168	24.100	-0.239	1.00	0.00		3A4
ATOM	2477	CG	MET	357	29.601	25.250	0.627	1.00	0.00		3A4

ATOM	2478	SD	MET	357	30	. 612	26.763	0.66	5 1.00	0.00	3A4
ATOM	2479	CE	MET	357	29	.381	27.754	1.56	2 1.00	0.00	3A4
ATOM	2480	С	MET	357	29	. 62 <b>2</b>	21.737	0.28	9 1.00	0.00	3A4
ATOM	2481	0	MET	357	28	.618	21.519	0.95		0.00	3A4
ATOM	2482	N	VAL	358		. 995	20.909	-0.71			3A4
MOTA	2483	CA	VAL	358		.302	19.693	-1.09			3A4
MOTA	2484	CB	VAL	358		.848	19.071	-2.37			3A4
ATOM	2485		VAL	358		.224	17.667	-2.68			3A4
MOTA	2486		VAL	358		.530	20.074	-3.45			3A4
ATOM	2487	С	VAL	358		.376	18.671	0.01			3A4 3A4
MOTA	2488	0	VAL	358		.364	18.076	0.36			3A4
ATOM	2489	N	VAL	359		.567 .783	18.479 17.579	1.75			3A4
ATOM	2490 2491	CA CB	VAL VAL	359 359		. 264	17.531	2.14			3A4
MOTA MOTA	2492		VAL	359		.553	16.768	3.45			3A4
ATOM	2493		VAL	359		.043	16.854	1.00			3A4
ATOM	2494	c	VAL	359		.954	17.977	2.96			3A4
ATOM	2495	ŏ	VAL	359		.303	17.151	3.59		0.00	3A4
ATOM	2496	N	ASN	360		.903	19.287	3.26	3 1.00	0.00	3A4
ATOM	2497	CA	ASN	360	29	.117	19.830	4.35	0 1.00	0.00	3A4
MOTA	2498	CB	ASN	360	29	.412	21.328	4.53	7 1.00		3A4
MOTA	2499	CG	ASN	360	30	.795	21.548	5.18			3A4
ATOM	2500		ASN	360		.725	20.750	5.08			3A4
ATOM	2501		ASN	360		.946	22.706	5.89			3A4
MOTA	2502	С	ASN	360		.624	19.645	4.14			3A4 3A4
ATOM	2503	0	ASN	360		.891	19.274	5.06 2.89			3A4
ATOM	2504	N CA	GLU GLU	361 361		.768	19.820 19.606	2.52			3A4
ATOM ATOM	2505 2506	CB	GLU	361		.458	20.211	1.13			3A4
ATOM	2507	CG	GLU	361		.026	19.998	0.62			3A4
ATOM	2508	CD	GLU	361		.935	20.638	1.48			3A4
ATOM	2509		GLU	361		.253	21.306	2.50	4 1.00	0.00	3A4
ATOM	2510	OE2	GLU	361	21	.740	20.442	1.14			3A4
MOTA	2511	C	GLU	361		. 372	18.147	2.55			3A4
ATOM	2512	0	GLU	361		.258	17.809	2.94			3A4
ATOM	2513	N	THR	362		.285	17.210	2.20			3A4 3A4
ATOM ATOM	2514 2515	CA CB	THR THR	362 362		.034	14.973	1.57			3A4
ATOM	2516		THR	362		.154	15.360	0.20			3A4
ATOM	2517		THR	362		.766	13.462	1.67			3A4
ATOM	2518	С	THR	362		.886	15.303	3.70	2 1.00	0.00	3A4
ATOM	2519	0	THR	362	24	.990	14.527	4.02			
ATOM	2520	N	LEU	363		.722	15.835	4.61			
ATOM	2521	CA	LEU	363		. 677	15.555	6.02			
ATOM	2522	CB	LEU	363		.934	16.102	6.72			
ATOM	2523	CG	LEU	363		.216	15.310	6.42 6.74			
ATOM ATOM	2524 2525		LEU	363 363		.434	16.188 13.981	7.21			
ATOM	2526	C	LEU	363		.448	16.157	6.69			
MOTA	2527	ŏ	LEU	363		.956	15.614	7.68			
ATOM	2528	N	ARG	364		.890	17.274	6.16	3 1.00	0.00	3A4
ATOM	2529	CA	ARG	364	23	.659	17.879	6.63			
MOTA	2530	СВ	ARG	364		.446	19.303	6.08			
ATOM	2531	CG	ARG	364		.238		6.67			
ATOM	2532	CD	ARG	364		.212	21.544	6.41			
ATOM	2533	NE	ARG	364		.256	22.182	7.39 8.59			
MOTA	2534	CZ	ARG	364		.624	22.741 23.251	9.41			
ATOM ATOM	2535 2536		ARG ARG	364 364		.925	22.809	8.99			
ATOM	2537	C	ARG	364		.463	17.060	6.23			
ATOM	2538	ŏ	ARG	364		. 622	16.711	7.04			
ATOM	2539	N	LEU	365	22	.393	16.685	4.94	0 1.00	0.00	3A4
ATOM	2540	CA	LEU	365		.267	15.979	4.38	1.00		
ATOM	2541	СВ	LEU	365		.247	16.050	2.84			
ATOM	2542	CG	LEU	365		.879	16.592	2.32			
MOTA	2543		LEU	365		.837	16.585	0.81			
ATOM	2544		LEU	365 365		.607	15.874	2.82			
ATOM ATOM	2545 2546	С О	LEU LEU	365 365		.029	14.540	4.81 5.08	_		
ATOM	2546 2547	N	PHE	366		.252	13.787	4.90			and the second s
ATOM	2548	CA	PHE	366		.226	12.409	5.37			
ATOM	2549	СВ	PHE	366		.642	11.385	4.27			

ATOM	2550	CG	PHE	366	21.503	11.244	3.297	1.00	0.00	3A4
ATOM	2551	CD1		366	21.538	11.861	2.035	1.00	0.00	3A4
MOTA	2552	CD2		366	20.363	10.498	3.651	1.00	0.00	3A4
MOTA	2553	CE1	PHE	366	20.455	11.742	1.150	1.00	0.00	3A4
MOTA	2554	CE2	PHE	366	19.278	10.377	2.773	1.00	0.00	3A4
MOTA	2555	CZ	PHE	366	19.325	11.000	1.520	1.00	0.00	3A4
ATOM	2556	С	PHE	366	23.116	12.273	6.585	1.00	0.00	3A4 3A4
MOTA	2557	0	PHE	366	24.165	11.637	6.497	1.00	0.00	3A4
ATOM	2558	N	PRO	367	22.732	12.795	7.772 9.011	1.00	0.00	3A4
ATOM	2559	CA	PRO	367	23.466 21.498	12.674 13.517	7.993	1.00	0.00	3A4
ATOM	2560	CD CB	PRO PRO	367 367	22.894	13.739	9.935	1.00	0.00	3A4
ATOM ATOM	2561 2562	CG	PRO	367	21.461	13.878	9.463	1.00	0.00	3A4
ATOM	2563	C	PRO	367	23.332	11.269	9.536	1.00	0.00	3A4
ATOM	2564	ŏ	PRO	367	22.246	10.779	9.824	1.00	0.00	3A4
ATOM	2565	N	ILE	368	24.476	10.572	9.569	1.00	0.00	3A4
ATOM	2566	CA	ILE	368	24.602	9.143	9.718	1.00	0.00	3A4
ATOM	2567	CB	ILE	368	25.992	8.818	9.131	1.00	0.00	3A4
ATOM	2568	CG2	ILE	368	27.160	9.306	10.024	1.00	0.00	3A4
ATOM	2569		ILE	368	26.230	7.413	8.553	1.00	0.00	3A4 3A4
ATOM	2570	CD	ILE	368	26.421	6.268	9.546	1.00	0.00	3A4
ATOM	2571	C	ILE	368	24.406	8.654	11.153	1.00	0.00	3A4
ATOM	2572	0	ILE	368	24.024	7.515 9.530	11.392 12.146	1.00	0.00	3A4
MOTA	2573	N	ALA	369	24.661 24.719	9.183	13.542	1.00	0.00	3A4
ATOM	2574	CA CB	ALA ALA	369 369	26.067	9.640	14.141	1.00	0.00	3A4
ATOM ATOM	2575 2576	С	ALA	369	23.654	9.859	14.360	1.00	0.00	3A4
ATOM	2577	Ö	ALA	369	23.267	10.991	14.104	1.00	0.00	3A4
ATOM	2578	N	MET	370	23.265	9.221	15.511	1.00	0.00	3A4
ATOM	2579	CA	MET	370	22.422	9.803	16.560	1.00	0.00	3A4
ATOM	2580	СВ	MET	370	20.964	9.264	16.470	1.00	0.00	3A4
MOTA	2581	CG	MET	370	19.910	10.113	17.209	1.00	0.00	· 3A4
MOTA	2582	SD	MET	370	18.173	9.663	16.885	1.00	0.00	3A4
MOTA	2583	CE	MET	370	18.081	10.195	15.146	1.00	0.00	3A4
ATOM	2584	С	MET	370	23.062	9.512	17.921	1.00	0.00 0.00	3A4 3A4
ATOM	2585	0	MET	370	23.884	8.603 10.299	18.029 18.992	1.00 1.00	0.00	3A4
ATOM	2586	N	ARG	371	22.711 23.356	10.233	20.307	1.00	0.00	3A4
ATOM	2587 2588	CA CB	ARG ARG	371 371	24.430	11.405	20.437	1.00	0.00	3A4
ATOM ATOM	2589	CG	ARG	371	23.944	12.828	20.099	1.00	0.00	3A4
ATOM	2590	CD	ARG	371	25.049	13.888	20.216	1.00	0.00	· 3A4
ATOM	2591	NE	ARG	371	24.503	15.208	19.738	1.00	0.00	3A4
ATOM	2592	CZ	ARG	371	25.012	16.428	20.108	1.00	0.00	3A4
MOTA	2593	NH1	ARG	371	24.468	17.561	19.575	1.00	0.00	3A4
MOTA	2594	NH2	ARG	371	26.049	16.546	20.988	1.00	0.00	3A4
MOTA	2595	С	ARG	371	22.333	10.392	21.438	1.00	0.00	3A4
MOTA	2596	0	ARG	. 371	21.181	10.760	21.216	1.00	0.00	3A4 3A4
	2597	N	LEU	372	22.776	10.045	22.692	1.00	0.00 0.00	3A4 3A4
ATOM	2598	CA	LEU	372.	22.016	9.951 8.482	23.936 24.512	1.00	0.00	3A4
MOTA	2599 2600	CB CG	LEU	372 372	21.964 21.345	7.343	23.661	1.00	0.00	3A4
ATOM ATOM	2601		LEU	372	19.908	7.641	23.227	1.00	0.00	3A4
ATOM	2602		LEU	372	22.216	6.816	22.501	1.00	0.00	3A4
ATOM	2603	c	LEU	372	22.693	10.771	25.005	1.00	0.00	3A4
ATOM	2604	ō	LEU	372	23.899	11.003	24.975	1.00	0.00	3A4
ATOM	2605	N	GLU	373	21.900	11.155	26.021	1.00	0.00	3A4
MOTA	2606	CA	GLU	373	22.322	11.807	27.237	1.00	0.00	3A4
ATOM	2607	СB	GLU	373	22.131	13.344	27.172	1.00	0.00	3A4
ATOM	2608	CG	GLU	373	23.197	14.057	26.329	1.00	0.00	3A4 3A4
ATOM	2609	CD	GLU	373	23.009	15.577	26.343	1.00	0.00	3A4
MOTA	2610		GLU	373	23.722	16.250 16.090	25.553 27.128	1.00	0.00	3A4
ATOM	2611	OE2		373 373	22.167 21.466	11.241	28.351	1.00	0.00	3A4
ATOM	2612	C	GLU GLU	373 373	20.387	10.695	28.121	1.00	0.00	3A4
MOTA MOTA	2613 2614	O N	ARG	374	21.930	11.386	29.612	1.00	0.00	3A4
ATOM	2615	CA	ARG	374	21.138	11.043	30.774	1.00	0.00	3A4
ATOM	2616	СВ	ARG	374	21.532	9.678	31.420	1.00	0.00	3A4
MOTA	2617	CG	ARG	374	22.371	9.595	32.715	1.00	0.00	3A4
ATOM	2618	CD	ARG	374	21.558	9.546	34.018	1.00	0.00	3A4
ATOM	2619	NE	ARG	374	22.476	9.916	35.152	1.00	0.00	3A4
ATOM	2620	CZ	ARG	374	22.249	9.595	36.465	1.00	0.00	3A4
ATOM	2621	NHl	ARG	374	23.147	10.010	37.405	1.00	0.00	3A4

ATOM	2622	NH2	ARG	374	21.156	8.879	36.860	1.00	0.00	3A4
ATOM	2623	С	ARG	374	21.272	12.200	31.721	1.00	0.00	3A4
ATOM	2624	0	ARG	374	22.360	12.720	31.947	1.00	0.00	3A4
ATOM	2625	N	VAL	375	20.152	12.629	32.340	1.00	0.00	3A4
ATOM	2626	CA	VAL	375	20.085	13.742	33.272	1.00	0.00	3A4 3A4
ATOM	2627	CB	VAL	375	18.651	14.239	33.344	1.00 1.00	0.00	3A4
ATOM	2628	CG1 CG2		375 375	18.283 18.394	15.175 14.888	34.420 31.964	1.00	0.00	3A4
ATOM	2629 2630	C	VAL	375	20.606	13.314	34.625	1.00	0.00	3A4
ATOM ATOM	2631	ŏ	VAL	375	20.173	12.325	35.197	1.00	0.00	3A4
ATOM	2632	N	CYS	376	21.593	14.058	35.166	1.00	0.00	3A4
ATOM	2633	CA	CYS	376	22.269	13.722	36.404	1.00	0.00	3A4
ATOM	2634	СВ	CYS	376	23.708	14.284	36.408	1.00	0.00	3A4
ATOM	2635	SG	CYS	376	24.721	13.423	35.165	1.00	0.00	3A4
ATOM	2636	С	CYS	376	21.525	14.230	37.618	1.00	0.00	. 3A4
MOTA	2637	0	CYS	376	21.699	13.713	38.720	1.00	0.00	3A4
ATOM	2638	N	LYS	377	20.691	15.268	37.426	1.00 1.00	0.00 0.00	3A4 3A4
ATOM	2639	CA	LYS	377 377	19.982 20.773	15.944 17.167	38.480 38.996	1.00	0.00	3A4
ATOM ATOM	2640 2641	CB CG	LYS LYS	377	22.008	16.876	39.867	1.00	0.00	3A4
ATOM	2642	CD	LYS	377	21.695	16.179	41.198	1.00	0.00	3A4
ATOM	2643	CE	LYS	377	22.947	15.957	42.056	1.00	0.00	3A4
ATOM	2644	NZ	LYS	377	22.604	15.293	43.336	1.00	0.00	3A4
ATOM	2645	С	LYS	377	18.735	16.448	37.827	1.00	0.00	3A4
ATOM	2646	0	LYS	377	18.689	16.603	36.617	1.00	0.00	3A4
ATOM	2647	N	LYS	378	17.690	16.839	38.593	1.00	0.00	3A4
ATOM	2648	CA	LYS	378	16.465	17.414	38.063	1.00	0.00	3A4
MOTA	2649	СВ	LYS	378	15.419	17.607	39.177	1.00	0.00 0.00	3A4 3A4
MOTA	2650	CG	LYS	378 378	15.088 14.017	16.287 16.418	39.895 40.984	1.00	0.00	3A4
ATOM ATOM	2651 2652	CD	LYS LYS	378	13.613	15.082	41.625	1.00	0.00	3A4
MOTA	2653	NZ	LYS	378	14.747	14.462	42.352	1.00	0.00	3A4
ATOM	2654	C	LYS	378	16.741	18.741	37.382	1.00	0.00	3A4
ATOM	2655	0	LYS	378	17.545	19.524	37.877	1.00	0.00	3A4
ATOM	2656	N	ASP	379	16.172	18.960	36.183	1.00	0.00	3A4
MOTA	2657	CA	ASP	379	16.483	20.125	35.394	1.00	0.00	3A4
ATOM	2658	СВ	ASP	379	17.706	19.925	34.443	1.00	0.00	3A4
ATOM	2659	CG	ASP	379	17.527	19.059	33.183	1.00	0.00	3A4 3A4
ATOM	2660		ASP	379	17.455 17.475	17.817 19.634	33.330 32.063	1.00	0.00	3A4
ATOM ATOM	2661 2662	C	ASP ASP	379 379	15.250	20.543	34.652	1.00	0.00	3A4
MOTA	2663	ŏ	ASP	379	14.333	19.776	34.415	1.00	0.00	3A4
ATOM	2664	N	VAL	380	15.216	21.819	34.247	1.00	0.00	3A4
ATOM	2665	CA	VAL	380	14.098	22.398	33.548	1.00	0.00	3A4
ATOM	2666	СВ	VAL	380	13.450	23.491	34.376	1.00	0.00	3A4
ATOM	2667		VAL	380	12.212	24.040	33.665	1.00	0.00	3A4
ATOM	2668		VAL	380	13.057	22.943	35.763	1.00	0.00	3A4
MOTA	2669	C	VAL	380	14.659	22.869	32.227	1.00	0.00	3A4 3A4.
ATOM	2670 2671	N O	VAL	380 381	15.521 14.219	23.743 22.259	32.201 31.107	1.00	0.00	3A4
ATOM ATOM	2672	CA	GLU GLU	381	14.653	22.560	29.760	1.00	0.00	3A4
ATOM	2673	СВ	GLU	381	15.044	21.298	28.989	1.00	0.00	3A4
ATOM	2674	CG	GLU	381	15.995	21.611	27.810	1.00	0.00	3A4 `
MOTA	2675	CD	GLU	381	16.331	20.375	26.965	1.00	0.00	3A4
ATOM	2676		GLU	381	17.063	20.564	25.958	1.00	0.00	3A4
MOTA	2677		GLÜ	381	15.873	19.246	27.284	1.00	0.00	3A4
MOTA	2678	C	GLU	381	13.495	23.231	29.052	1.00	0.00	3A4 3A4
MOTA	2679	0	GLU	381	12.355	22.802 24.405	29.042 28.468	1.00	0.00	3A4
MOTA MOTA	2680 2681	N CA	ILE	382 382	13.715 12.690	25.313	27.960	1.00	0.00	3A4
MOTA	2682	CB	ILE	382	11.956	24.945	26.638	1.00	0.00	3A4
MOTA	2683		ILE	382	10.525	25.549	26.472	1.00	0.00	3A4
ATOM	2684		ILE	382	12.874	25.434	25.467	1.00	0.00	3A4
ATOM	2685	CD	ILE	382	12.229	25.497	24.082	1.00	0.00	3A4
MOTA	2686	С	ILE	382	11.919	25.809	29.163	1.00	0.00	3A4
MOTA	2687	0	ILE	382	12.497	26.469	29.990	1.00	0.00	3A4
ATOM	2688	N	ASN	383	10.722	25.435	29.490	1.00	0.00	3A4 3A4
ATOM	2689	CA	ASN	383 383	10.349 9.806	25.838 27.330	30.866 30.959	1.00	0.00	3A4
ATOM	2690 2691	CB CG	ASN ASN	383 383	9.693	27.860	30.939	1.00	0.00	3A4
ATOM ATOM	2691		ASN	383	8.596	28.169	32.869	1.00	0.00	3A4
MOTA	2693		ASN	383	10.843	27.967	33.129	1.00	0.00	3A4

ATOM	2694	С	ASN	383	9.349	24.945	31.284	1.00	0.00	3A4
ATOM	2695	0	ASN	383	8.160	25.107	30.993	1.00	0.00	3A4
MOTA	2696	N	GLY	384	9.485	23.892	32.102	1.00	0.00	3A4
MOTA	2697	CA	GLY	384	8.315	22.984	32.156	1.00	0.00	3A4
ATOM	2698	С	GLY	384	8.276	22.292	30.798	1.00	0.00	3A4 3A4
ATOM	2699	0	GLY	384	7.285	21.764	30.297	1.00	0.00	3A4
ATOM	2700	N	MET	385	9.600 9.904	22.252 20.858	30.331 30.491	1.00 1.00	0.00	3A4
ATOM	2701 2702	CA CB	MET MET	385 385	10.648	20.838	29.245	1.00	0.00	3A4
MOTA MOTA	2702	CG	MET	385	10.078	18.932	28.749	1.00	0.00	3A4
ATOM	2704	SD	MET	385	10.271	17.522	29.885	1.00	0.00	3A4
ATOM	2705	CE	MET	385	8.674	16.747	29.504	1.00	0.00	3A4
ATOM	2706	С	MET	385	10.673	20.574	31.772	1.00	0.00	3A4
MOTA	2707	0	MET	385	11.823	20.957	31.867	1.00	0.00	3A4
ATOM	2708	N	PHE	386	10.077	19.903	32.767	1.00	0.00	3A4
ATOM	2709	CA	PHE	386	10.786	19.416	33.933	1.00	0.00	3A4 3A4
ATOM	2710	CB	PHE	386	9.854	19.471	35.160 36.492	1.00	0.00	3A4 3A4
ATOM	2711	CG	PHE	386 386	10.561 10.905	19.327 20.467	37.242	1.00	0.00	3A4
ATOM ATOM	2712 2713		PHE	386	10.861	18.057	37.026	1.00	0.00	3A4
ATOM	2714		PHE	386	11.556	20.349	38.477	1.00	0.00	3A4
ATOM	2715		PHE	386	11.512	17.931	38.260	1.00	0.00	3A4
MOTA	2716	CZ	PHE	386	11.859	19.080	38.985	1.00	0.00	3A4
ATOM	2717	С	PHE	386	11.245	17.997	33.650	1.00	0.00	3A4
ATOM	2718	0	PHE	386	10.434	17.097	33.442	1.00	0.00	3A4
MOTA	2719	N	ILE	387	12.579	17.797	33.622	1.00	0.00	3A4
ATOM	2720	CA	ILE	387	13.234	16.542	33.348	1.00	0.00	3A4
ATOM	2721	CB	ILE	387	14.381	16.682 15.256	32.335	1.00	0.00	3A4 3A4
ATOM	2722 2723		ILE	387 387	14.760 13.940	17.566	31.874 31.142	1.00	0.00	3A4
ATOM ATOM	2724	CD	ILE	387	14.996	17.732	30.052	1.00	0.00	3A4
ATOM	2725	c	ILE	387	13.712	16.037	34.699	1.00	0.00	3A4
MOTA	2726	ō	ILE	387	14.542	16.701	35.311	1.00	0.00	3A4
MOTA	2727	N	PRO	388	13.230	14.898	35.231	1.00	0.00	3A4
ATOM	2728	CA	PRO	388	13.741	14.297	36.449	1.00	0.00	3A4
ATOM	2729	CD	PRO	388	11.827	14.522	35.038	1.00	0.00	3A4
ATOM	2730	СВ	PRO	388	12.685	13.264	36.864	1.00	0.00	3A4 3A4
ATOM	2731	CG	PRO	388	11.381 15.090	13.833 13.656	36.327 36.297	1.00	0.00	3A4
ATOM ATOM	2732 2733	0	PRO PRO	388 388	15.481	13.036	35.212	1.00	0.00	3A4
ATOM	2734	N	LYS	389	15.825	13.516	37.416	1.00	0.00	3A4
ATOM	2735	CA	LYS	389	17.102	12.839	37.479	1.00	0.00	3A4
ATOM	2736	СВ	LYS	389 -	17.661	12.891	38.918	1.00	0.00	3A4
ATOM	2737	ÇG	LYS	389	16.754	12.453	40.092	1.00	0.00	3A4
MOTA	2738	CD	LYS	389	16.878	10.984	40.532	1.00	0.00	3A4
MOTA	2739	CE	LYS	389	16.079	10.653	41.802	1.00	0.00	3A4
MOTA	2740	NZ	LYS	389	14.624	10.849	41.589	1.00	0.00	3A4 3A4
ATOM ATOM	2741 2742	С 0	LYS LYS	389 389	16.984 15.997	11.412 10.745	37.009 37.301	1.00	0.00	3A4
ATOM	2742	N	GLY	390	17.932	10.973	36.172	1.00	0.00	3A4
ATOM	2744	CA	GLY	390	17.963	9.654	35.593	1.00	0.00	3A4
ATOM	2745	C	GLY	390	17.174	9.470	34.332	1.00	0.00	3A4
ATOM	2746	0	GLY	390	17.046	8.351	33.839	1.00	0.00	3A4
MOTA	2747	N	TRP	391	16.619	10.571	33.769	1.00	0.00	3A4
ATOM	2748	CA	TRP	391	15.850	10.544	32.546	1.00	0.00	3A4
ATOM	2749	СВ	TRP	391	14.930	11.760	32.448	1.00	0.00	3A4
ATOM	2750	CG	TRP	391	13.571	11.608	33.100	1.00	0.00	3A4 3A4
ATOM ATOM	2751 2752		TRP TRP	391 391	13.050 12.458	10.792 12.068	34.187 32.439	1.00	0.00	3A4
ATOM	2753		TRP	391	11.305	11.618	33.025	1.00	0.00	3A4
ATOM	2754		TRP	391	11.634	10.839	34.102	1.00	0.00	3A4
ATOM	2755		TRP	391	13.655	10.032	35.188	1.00	0.00	'3A4
ATOM	2756		TRP	391	10.825	10.153	35.005	1.00	0.00	3A4
ATOM	2757		TRP	391	12.843	9.345	36.102	1.00	0.00	3A4
ATOM	2758		TRP	391	11.446	9.404	36.011	1.00	0.00	3A4
ATOM	2759	C	TRP	391	16.783	10.563	31.369	1.00	0.00	3A4
MOTA	2760	0	TRP	391	17.769	11.289	31.371	1.00	0.00	3A4 3A4
ATOM	2761 2762	N CA	VAL VAL	392 392	16.466 17.263	9.736 9.564	30.350 29.159	1.00	0.00	3A4
ATOM ATOM	2762	CB	VAL	392	17.203	8.105	28.700	1.00	0.00	3A4
ATOM	2764		VAL	392	17.957	7.898	27.322	1.00	0.00	3A4
ATOM	2765		VAL	392	17.984	7.270	29.787	1.00	0.00	3A4

ATOM	2766	С	VAL	392	16.723	10.497	28.110	1.00	0.00	3A4
MOTA	2767	0	VAL	392	15.519	10.598	27.908	1.00	0.00	3A4
ATOM	2768	N	VAL	393 393	17.636	11.234 12.226	27.453 26.455	1.00	0.00	3A4 3A4
MOTA MOTA	2769 2770	CA CB	VAL VAL	393	17.333 17.828	13.610	26.868	1.00	0.00	3A4
ATOM	2771		VAL	393	17.556	14.652	25.780	1.00	0.00	3A4
MOTA	2772	CG2	VAL	393	17.145	14.023	28.194	1.00	0.00	3A4
MOTA	2773	C	VAL	393	17.993	11.735	25.192	1.00	0.00	3A4
MOTA	2774	0	VAL	393	19.147	11.327	25.196	1.00	0.00	3A4
ATOM ATOM	2775 2776	N CA	MET MET	394 394	17.251 17.726	11.776 11.439	24.072 22.757	1.00	0.00	3A4 3A4
ATOM	2777	СВ	MET	394	16.799	10.393	22.065	1.00	0.00	3A4
ATOM	2778	CG	MET	394	16.558	9.106	22.860	1.00	0.00	3A4
ATOM	2779	SD	MET	394	15.673	7.800	21.946	1.00	0.00	3A4
ATOM	2780	CE	MET	394	16.910	7.426 12.724	20.666 21.991	1.00	0.00	3A4 3A4
MOTA MOTA	2781 2782	с 0	MET MET	394 394	17.772 16.799	13.464	21.937	1.00	0.00	3A4
ATOM	2783	N	ILE	395	18.916	13.023	21.347	1.00	0.00	3A4
ATOM	2784	CA	ILE	395	19.139	14.208	20.554	1.00	0.00	3A4
ATOM	2785	СВ	ILE	395	20.476	14.837	20.956	1.00	0.00	3A4
ATOM	2786	CG2		395	21.095	15.840	19.965	1.00	0.00	3A4 3A4
MOTA MOTA	2787 2788	CG1	ILE	395 395	20.413 20.802	15.442 14.496	22.374 23.518	1.00	0.00	3A4
ATOM	2789	c	ILE	395	19.146	13.747	19.102	1.00	0.00	3A4
ATOM	2790	0	ILE	395	20.160	13.239	18.627	1.00	0.00	3A4
MOTA	2791	N	PRO	396	18.048	13.907	18.342	1.00	0.00	3A4
ATOM	2792	CA	PRO	396	18.027 16.755	13.792	16.906	1.00	0.00	3A4 3A4
ATOM ATOM	2793 2794	CD CB	PRO PRO	396 396	16.531	13.448 13.829	18.870 16.546	1.00	0.00	3A4
ATOM	2795	CG	PRO	396	15.857	13.097	17.687	1.00	0.00	3A4
MOTA	2796	С	PRO	396	18.776	14.889	16.173	1.00	0.00	3A4
MOTA	2797	0	PRO	396	18.239	15.950	15.861	1.00	0.00	3A4
ATOM ATOM	2798 2799	N CA	SER SER	397 397	20.048 20.904	14.601 15.470	15.825 15.055	1.00	0.00	3A4 3A4
MOTA	2800	CB	SER	397	22.360	14.989	15.079	1.00	0.00	3A4
ATOM	2801	OG	SER	397	22.500	13.601	14.800	1.00	0.00	3A4
MOTA	2802	С	SER	397	20.417	15.595	13.635	1.00	0.00	3A4
ATOM	2803	0	SER	397	20.522	16.640	13.023	1.00	0.00	3A4
ATOM ATOM	2804 2805	N CA	TYR TYR	398 398	19.766 19.026	14.539 14.496	13.106 11.862	1.00	0.00	3A4 3A4
ATOM	2806	СВ	TYR	398	18.323	13.079	11.799	1.00	0.00	3A4
ATOM	2807	CG	TYR	398	18.447	12.353	10.483	1.00	0.00	3A4
ATOM	2808	CD1		398	19.004	11.056	10.456	1.00	0.00	3A4
ATOM	2809	CD2		398	18.041	12.935	9.266 9.251	1.00	0.00	3A4
ATOM ATOM	2810 2811	CE1	TYR	398 398	19.153 18.216	10.357 12.249	8.058	1.00 1.00	0.00	3A4 3A4
ATOM	2812	CZ	TYR	398	18.763	10.958	8.048	1.00	0.00	3A4
ATOM	2813	OH	TYR	398	18.924	10.266	6.829	1.00	0.00	3A4
ATOM	2814	С	TYR	398	17.923	15.540	11.741	1.00	0.00	3A4
ATOM ATOM	2815 2816	O N	TYR ALA	398 399	17.730 17.184	16.207 15.730	10.728 12.853	1.00	0.00	3A4 3A4
ATOM	2817	CA	ALA	399	16.116	16.686	12.969	1.00	0.00	3A4
MOTA	2818	СВ	ALA	399	15.263	16.409	14.206	1.00	0.00	3A4
ATOM	2819	С	ALA	399	16.594	18.122	13.028	1.00	0.00	3A4
ATOM ATOM	2820 2821	N N	ALA LEU	399 400	15.939 17.795	19.008 18.377	12.501 13.599	1.00 1.00	0.00	3A4 3A4
ATOM	2822	CA	LEU	400	18.426	19.687	13.645	1.00	0.00	3A4
ATOM	2823	СВ	LEU	400	19.762	19.647	14.448	1.00	0.00	3A4
MOTA	2824	CG	LEU	400	19.694	19.664	15.956	1.00	0.00	3A4
ATOM	2825	CD1		400	20.663	20.773	16.433	1.00	0.00	3A4
ATOM ATOM	2826 2827	CD2 C	LEU	400 400	18.244 18.832	19.759 20.202	16.433 12.285	1.00 1.00	0.00	3A4 3A4
ATOM	2828	ò	LEU	400	18.639	21.368	11.954	1.00	0.00	3A4
MOTA	2829	N	HIS	401	19.402	19.298	11.465	1.00	0.00	3A4
ATOM	2830	CA	HIS	401	19.852	19.556	10.124	1.00	0.00	3A4
MOTA MOTA	2831	ND1		401	22.332 21.917	16.943 18.117	10.714	1.00	0.00	3A4 3A4
ATOM	2832 2833	CG CB	HIS HIS	401 401	20.572	18.117	10.143 9.559	1.00	0.00	3A4
ATOM	2834	NE2		401	24.123	18.219	10.505	1.00	0.00	3A4
MOTA	2835	CD2	HIS	401	23.023	18.893	10.033	1.00	0.00	3A4
ATOM	2836	CE1		401	23.659	17.057	10.914	1.00	0.00	3A4
MOTA	2837	С	HIS	401	18.745	19.836	9.125	1.00	0.00	3A4

MOTA	2838	0	HIS	401	18.970	20.398	8.056	1.00	0.00	3A4
MOTA	2839	N	ARG	402	17.513	19.410	9.474	1.00	0.00	3A4
MOTA	2840	CA	ARG	402	16.350	19.558	8.644	1.00	0.00	3A4 3A4
MOTA	2841	CB	ARG	402 402	15.632 16.476	18.220 17.220	8.410 7.607	1.00	0.00	3A4
MOTA	2842	CG CD	ARG ARG	402	15.663	15.992	7.176	1.00	0.00	3A4
MOTA MOTA	2843 2844	NE	ARG	402	16.519	15.105	6.308	1.00	0.00	3A4
ATOM	2845	CZ	ARG	402	16.028	14.373	5.254	1.00	0.00	3A4
ATOM	2846	NH1	ARG	402	16.860	13.518	4.593	1.00	0.00	3A4
ATOM	2847	NH2		402	14.725	14.465	4.853	1.00	0.00	3A4 3A4
MOTA	2848	С	ARG	402	15.378	20.553	9.211 8.790	1.00	0.00 0.00	3A4
ATOM	2849	0	ARG ASP	402 403	14.224 15.839	21.391	10.171	1.00	0.00	3A4
MOTA MOTA	2850 2851	N CA	ASP	403	15.031	22.422	10.772	1.00	0.00	3A4
ATOM	2852	СВ	ASP	403	15.642	22.973	12.085	1.00	0.00	3A4
ATOM	2853	CG	ASP	403	14.530	23.734	12.847	1.00	0.00	3A4
ATOM	2854		ASP	403	14.116	24.806	12.394	1.00	0.00	3A4 3A4
ATOM	2855		ASP	403	13.981	23.160	13.823 9.771	1.00	0.00	3A4
ATOM	2856	C	ASP	403 403	14.822 15.805	23.549 24.148	9.348	1.00	0.00	3A4
ATOM ATOM	2857 2858	O N	ASP PRO	404	13.575	23.872	9.387	1.00	0.00	3A4
ATOM	2859	CA	PRO	404	13.256	24.866	8.377	1.00	0.00	3A4
ATOM	2860	CD	PRO	404	12.350	23.288	9.945	1.00	0.00	3A4
MOTA	2861	CB	PRO	404	11.749	24.727	8.133	1.00	0.00	3A4
MOTA	2862	CG	PRO	404	11.195	24.161	9.445 8.784	1.00	0.00	3A4 3A4
ATOM	2863	C	PRO	404	13.582 13.786	26.287 27.122	7.915	1.00	0.00	3A4
ATOM	2864 2865	О И	PRO Lys	404 405	13.702	26.594	10.092	1.00	0.00	3A4
ATOM ATOM	2866	CA	LYS	405	14.102	27.890	10.588	1.00	0.00	3A4
ATOM	2867	СВ	LYS	405	13.708	28.082	12.078	1.00	0.00	3A4
ATOM	2868	CG	LYS	405	12.230	27.779	12.361	1.00	0.00	3A4
ATOM	2869	CD	LYS	405	11.862	27.931	13.843	1.00	0.00	3A4 3A4
MOTA	2870	CE	LYS	405	10.437 9.420	27.465 28.274	14.181 13.467	1.00	0.00	3A4
ATOM	2871 2872	NZ C	LYS LYS	405 405	15.589	28.111	10.451	1.00	0.00	3A4
ATOM ATOM	2873	ò	LYS	405	16.040	29.247	10.435	1.00	0.00	3A4
MOTA	2874	N	TYR	406	16.387	27.031	10.326	1.00	0.00	3A4
ATOM	2875	CA	TYR	406	17.828	27.082	10.196	1.00	0.00	3A4
ATOM	2876	СВ	TYR	406	18.501	25.978	11.073 12.466	1.00	0.00	3A4 3A4
ATOM	2877	CG	TYR	406 406	18.818 17.845	26.481 27.049	13.316	1.00	0.00	3A4
ATOM ATOM	2878 2879		TYR TYR	406 406	20.123	26.324	12.973	1.00	0.00	3A4
MOTA	2880		TYR	406	18.180	27.502	14.601	1.00	0.00	3A4
ATOM	2881	CE2		406	20.465	26.758	14.261	1.00	0.00	3A4
ATOM	2882	CZ	TYR	406	19.493	27.354	15.076	1.00	0.00	3A4 3A4
ATOM	2883	ОН	TYR	406	19.831	27.781	16.379 8.742	1.00	0.00	3A4
ATOM	2884 2885	c o	TYR TYR	406 406	18.238 19.185	26.911 27.556	8.293	1.00	0.00	3A4
ATOM ATOM	2886	N	TRP	407	17.542	26.030	7.986	1.00	0.00	3A4
ATOM	2887	CA	TRP	407	17.869	25.728	6.609	1.00	0.00	3A4
ATOM	2888	СВ	TRP	407	18.602	24.364	6.460	1.00	0.00	3A4
ATOM	2889	CG	TRP	407	19.890	24.534	5.666	1.00	0.00	3A4 3A4
MOTA	2890		TRP	407	20.082 21.050	24.159 25.141	4.293 6.063	1.00	0.00	3A4
ATOM ATOM	2891 2892		TRP TRP	407 407	21.981	25.110	5.052	1.00	0.00	3A4
ATOM	2893		TRP	407	21.405	24.521	3.948	1.00	0.00	3A4
ATOM	2894		TRP	407	19.231	23.566	3.365	1.00	0.00	3A4
MOTA	2895		TRP	407	21.902	24.280	2.673	1.00	0.00	3A4 3A4
ATOM	2896		TRP	407	19.728	23.326	2.076 1.741	1.00	0.00	3A4
ATOM	2897		TRP	407 407	21.046 16.592	23.678 25.684	5.809	1.00	0.00	3A4
MOTA MOTA	2898 2899	С 0	TRP TRP	407	15.735	24.831	6.029	1.00	0.00	3A4
ATOM	2900	N	THR	408	16.454	26.581	4.791	1.00	0.00	3A4
ATOM	2901	CA	THR	408	15.311	26.691	3.895	1.00	0.00	3A4
MOTA	2902	CB	THR	408	15.211	28.071	3.263	1.00	0.00	3A4 3A4
MOTA	2903		THR	408	16.432	28.505 29.070	2.662 4.376	1.00		3A4 3A4
MOTA	2904		THR THR	408 408	14.818 15.392	25.598	2.839	1.00		3A4
MOTA MOTA	2905 2906	0	THR	408	16.472	25.245	2.376	1.00		3A4
MOTA	2907	N	GLU	409	14.235	24.987	2.499	1.00	0.00	3A4
MOTA	2908	CA	GLU	409	14.103	23.803	1.664	1.00		3A4
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ATOM	2910	CG	GLU	409	13.370	25.190	-0.379	1.00	0.00	3A4
ATOM	2911	CD	GLU	409	13.625	25.385	-1.878	1.00	0.00	3A4
MOTA	2912	OE1		409	12.698	25.099	-2.683	1.00	0.00	3A4 3A4
ATOM	2913	OE2		409 409	14.752 15.001	25.821 22.657	-2.236 2.097	1.00	0.00	3A4
ATOM ATOM	2914 2915	С 0	GLU	409	15.858	22.218	1.334	1.00	0.00	3A4
ATOM	2916	N	PRO	410	14.886	22.233	3.369	1.00	0.00	3A4
ATOM	2917	CA	PRO	410	15.857	21.388	4.073	1.00	0.00	3A4
ATOM	2918	ÇD	PRO	410	13.663	22.414	4.165	1.00	0.00	3A4 3A4
ATOM	2919	СВ	PRO	410	15.298	21.307 21.467	5.504 5.357	1.00	0.00	3A4
ATOM ATOM	2920 2921	CG C	PRO PRO	410 410	13.783 16.013	20.007	3.463	1.00	0.00	3A4
ATOM	2922	Ö	PRO	410	17.048	19.368	3.620	1.00	0.00	3A4
ATOM	2923	N	GLU	411	15.001	19.530	2.723	1.00	0.00	3A4
ATOM	2924	CA	GLU	411	15.007	18.249	2.086	1.00	0.00	3A4 3A4
ATOM	2925	СВ	GLU	411	13.575	17.671 18.662	2.041 1.868	1.00	0.00	3A4
ATOM ATOM	2926 2927	CG CD	GLU	411 411	12.398 12.395	19.342	0.498	1.00	0.00	3A4
ATOM	2928	OE1	GLU	411	12.459	20.600	0.464	1.00	0.00	3A4
ATOM	2929		GLU	411	12.316	18.616	-0.530	1.00	0.00	3A4
ATOM	2930	С	GLU	411	15.637	18.272	0.712	1.00	0.00	3A4 3A4
MOTA	2931	0	GLU	411	15.745	17.227 19.439	0.076 0.214	1.00	0.00	3A4
ATOM	2932 2933	N CA	LYS LYS	412 412	16.093 16.747	19.560	-1.069	1.00	0.00	3A4
MOTA MOTA	2934	CB	LYS	412	16.319	20.855	-1.798	1.00	0.00	3A4
ATOM	2935	CG	LYS	412	14.842	20.918	-2.228	1.00	0.00	3A4
MOTA	2936	CD	LYS	412	14.489	20.264	-3.577	1.00	0.00	3A4
ATOM	2937	CE	LYS	412	14.483	18.726	-3.601 -4.904	1.00	0.00	3A4 3A4
ATOM	2938 2939	NZ C	LYS LYS	412 412	13.990 18.246	18.220 19.556	-0.876	1.00	0.00	3A4
ATOM ATOM	2939	Ö	LYS	412	18.788	20.180	0.031	1.00	0.00	3A4
ATOM	2941	N	PHE	413	18.970	18.849	-1.771	1.00	0.00	3A4
MOTA	2942	CA	PHE	413	20.413	18.790	-1.784	1.00	0.00	3A4 3A4
ATOM	2943	CB	PHE	413	20.897	17.450 17.294	-2.401 -2.423	1.00	0.00	3A4
ATOM ATOM	2944 2945	CG CD1	PHE	413 413	22.398 23.168	17.227	-1.254	1.00	0.00	3A4
ATOM	2946		PHE	413	23.046	17.095	-3.661	1.00	0.00	3A4
ATOM	2947		PHE	413	24.550	16.999	-1.315	1.00	0.00	3A4
MOTA	2948		PHE	413	24.421	16.834	-3.726	1.00	0.00	3A4 3A4
ATOM	2949	cz	PHE	413	25.177	16.794 19.968	-2.550 -2.586	1.00	0.00	3A4
ATOM ATOM	2950 2951	С 0	PHE	413 413	20.891 20.724	20.009	-3.801	1.00	0.00	3A4
ATOM	2952	N	LEU	414	21.483	20.957	-1.901	1.00	0.00	3A4
ATOM	2953	CA	LEU	414	21.933	22.177	-2.522	1.00	0.00	3A4
ATOM	2954	СВ	LEU	414	20.902	23.301	-2.306	1.00	0.00	3A4 3A4
ATOM	2955	CG	LEU	414	21.169 21.261	24.700 24.685	-2.902 -4.441	1.00	0.00	3A4
ATOM ATOM	2956 2957		LEU	414 414	20.079	25.663	-2.388	1.00	0.00	3A4
ATOM	2958	C	LEU	414	23.275	22.553	-1.966	1.00	0.00	3A4.
ATOM	2959	0	LEU	414	23.343	23.031	-0.834	1.00	0.00	3A4
ATOM	2960	N	PRO	415	24.394	22.396	-2.681 -2.165	1.00	0.00	3A4 3A4
ATOM	2961 2962	CA CD	PRO PRO	415 415	25.721 24.457	22.710 21.932	-4.069	1.00	0.00	3A4
ATOM ATOM	2963	СВ	PRO	415	26.676	22.158	-3.227	1.00	0.00	3A4
ATOM	2964	CG	PRO	415	25.882	22.244	-4.535	1.00	0.00	3A4
MOTA	2965	С	PRO	415	25.978	24.200	-1.983	1.00	0.00	3A4 3A4
ATOM	2966	0	PRO	415	26.655 25.547	24.548 25.077	-1.013 -2.937	1.00	0.00	3A4
ATOM ATOM	2967 2968	N CA	GLU	416 416	25.810	26.505	-2.951	1.00	0.00	3A4
ATOM	2969	СВ	GLU	416	27.244	26.943	-3.438	1.00	0.00	3A4
MOTA	2970	CG	GLU	416	28.338	26.841	-2.361	1.00	0.00	3A4
MOTA	2971	CD	GLU	416	29.636	27.541	-2.784	1.00	0.00	3A4 3A4
ATOM	2972		GLU	416 416	29.584 30.704	28.756 26.872	-3.114 -2.759	1.00	0.00	3A4
MOTA • MOTA	2973 2974	C C	GLU	416	24.818	27.126	-3.902	1.00	0.00	3A4
ATOM	2975	ŏ	GLU	416	24.357	26.500	-4.855	1.00	0.00	3A4
ATOM	2976	N	ARG	417	24.555	28.429	-3.633	1.00	0.00	3A4
MOTA	2977	CA	ARG	417	23.940	29.448	-4.465 -5.229	1.00	0.00	3A4 3A4
ATOM	2978	CB CG	ARG ARG	417 417	22.623 21.420	29.089 28.657	-3.229	1.00	0.00	3A4
ATOM ATOM	2979 2980	CD	ARG		20.160	28.317	-5.191	1.00	0.00	3A4
MOTA	2981	NE	ARG		19.654	29.550	-5.895	1.00	0.00	3A4

	ATOM	2982	CZ	ARG	417	18.836	30.485	-5.308	1.00	0.00		3A4
•	ATOM	2983	NH1		417	18.453	31.575	-6.033	1.00	0.00		3A4 3A4
	ATOM ATOM	2984 2985	NH2 C	ARG ARG	417 417	18.396 23.675	30.357 30.614	-4.021 -3.534	1.00	0.00		3A4
	ATOM	2986	ŏ	ARG	417	23.277	31.695	-3.966	1.00	0.00		3A4
	ATOM	2987	N	PHE	418	23.883	30.380	-2.207	1.00	0.00		3A4
	MOTA	2988	CA	PHE	418	23.598	31.253	-1.087	1.00	0.00		3A4 3A4
	ATOM	2989 2990	CB CG	PHE PHE	418 418	22.842 23.400	30.493 29.109	0.064 0.354	1.00	0.00		3A4
	ATOM ATOM	2991	CD1		418	24.479	28.931	1.245	1.00	0.00		3A4
	ATOM	2992	CD2		418	22.845	27.967	-0.262	1.00	0.00		3A4
	MOTA	2993	CE1		418	25.002	27.653	1.496	1.00	0.00		3A4
	ATOM	2994	CE2	PHE PHE	418 418	23.361 24.442	26.688 26.532	-0.007 0.869	1.00	0.00		3A4 3A4
	ATOM ATOM	2995 2996	C	PHE	418	24.891	31.865	-0.589	1.00	0.00		3A4
	ATOM	2997	Ō	PHE	418	25.978	31.337	-0.822	1.00	0.00		3A4
	ATOM	2998	N	SER	419	24.764	33.010	0.130	1.00	0.00		3A4
	ATOM	2999	CA CB	SER SER	419 419	25.850 26.168	33.749 35.084	0.742 0.003	1.00	0.00		3A4 3A4
	MOTA MOTA	3000 3001	OG	SER	419	26.610	34.824	-1.323	1.00	0.00		3A4
	ATOM	3002	c	SER	419	25.419	34.042	2.158	1.00	0.00		3A4
	MOTA	3003	0	SER	419	24.254	33.869	2.516	1.00	0.00		3A4
	ATOM	3004	N CA	LYS	420 420	26.380 26.162	34.507 34.853	2.995 4.383	1.00	0.00		3A4 3A4
	MOTA ATOM	3005 3006	CB	LYS LYS	420	26.449	33.660	5.338	1.00	0.00		3A4
	ATOM	3007	CG	LYS	420	26.041	33.882	6.806	1.00	0.00		3A4
	ATOM	3008	CD	LYS	420	25.973	32.611	7.673	1.00	0.00		3A4 3A4
	ATOM	3009 3010	CE NZ	LYS	420 420	27.316 27.897	31.947 31.201	8.025 6.884	1.00 1.00	0.00 0.00		3A4
	ATOM ATOM	3011	C	LYS LYS	420	27.070	36.024	4.656	1.00	0.00		3A4
	ATOM	3012	ō	LYS	420	28.205	36.070	4.182	1.00	0.00		3A4
	ATOM	3013	N	LYS	421	26.554	37.018	5.432	1.00	0.00		3A4
	MOTA MOTA	3014 3015	CA CB	LYS LYS	421 421	27.150 26.041	38.319 39.410	5.697 5.739	1.00	0.00 0.00		3A4 3A4
	ATOM .		CG	LYS	421	26.518	40.872	5.751	1.00	0.00		3A4
	ATOM	3017	CD	LYS	421,	25.360	41.868	5.629	1.00	0.00		3A4
	ATOM	3018	CE	LYS	421	25.821	43.332	5.619	1.00	0.00		3A4
	ATOM ATOM	3019 3020	NZ C	LYS LYS	421 421	24.664 27.940	44.251 38.313	5.492 6.992	1.00	0.00 0.00		3A4 3A4
	ATOM	3021	Ö	LYS	421	28.871	39.099	7.165	1.00	0.00		3A4
	MOTA	3022	N	ASN	422	27.572	37.398	7.933	1.00	0.00		3A4
	MOTA	3023	CA	ASN	422	28.154	37.237	9.255	1.00	0.00		3A4 3A4
	ATOM ATOM	3024 3025	CB CG	ASN ASN	422 422	27.020 27.499	37.047 37.210	10.319 11.776	1.00	0.00 0.00		3A4
	ATOM	3026	OD1		422	27.456	36.260	12.556	1.00	0.00		3A4
	ATOM	3027	ND2		422	27.964	38.434	12.149	1.00	0.00		3A4
		3028	С	ASN	422	29.107	36.052	9.222	1.00	0.00		3A4 3A4
	MOTA MOTA	3029 3030	N N	ASN Lys	422 423	29.035 30.033	35.203 35.989	8.335 10.220	1.00	0.00		3A4
	ATOM	3031	CA	LYS	423	31.052	34.968	10.382	1.00	0.00	•	3A4
	MOTA	3032	СВ	LYS	423	32.450	35.576	10.704	1.00	0.00		3A4
	ATOM	3033 3034	CG	LYS	423	33.030 33.266	36.450 35.769	9.575 8.209	1.00	0.00 0.00		3A4 3A4
	ATOM ATOM	3035	CE	LYS LYS	423 423	34.431	34.762	8.142	1.00	0.00		3A4
	ATOM	3036	N2	LYS	423	34.107	33.470	8.794	1.00	0.00		3A4
	MOTA	3037	С	LYS	423	30.631	34.032	11.491	1.00	0.00		3A4
	ATOM	3038	0	LYS	423 424	30.939 29.907	34.245 32.953	12.663 11.101	1.00	0.00		3A4 3A4
	ATOM ATOM	3039 3040	N CA	ASP ASP	424	29.457	31.893	11.976	1.00	0.00		3A4
	ATOM	3041	СВ	ASP	424	28.060	32.147	12.651	1.00	0.00		3A4
	MOTA	3042	CG	ASP	424	26.909	32.519	11.687	1.00	0.00		3A4
	ATOM	3043 3044		ASP	424 424	25.944 26.973	31.714 33.604	11.589 11.051	1.00	0.00 0.00		3A4 3A4
	ATOM ATOM	3044	C	ASP ASP	424	29.495	30.648	11.123	1.00	0.00		3A4
	ATOM	3046	ō	ASP	424	28.470	30.043	10.811	1.00	0.00		3A4
	MOTA	3047	N	ASN	425	30.728	30.251	10.724	1.00	0.00		3A4 3A4
	MOTA	3048 3049	CA CB	ASN ASN	425 425	30.999 30.910	29.112 29.449	9.872 8.339	1.00	0.00 0.00		3A4 3A4
	MOTA MOTA	3050	CG	ASN	425	31.718	30.701	7.912	1.00	0.00		3A4
	MOTA	3051	OD1	ASN	425	32.894	30.588	7.570	1.00	0.00		3A4
	MOTA	3052		ASN	425	31.085	31.907	7.916	1.00	0.00		3A4
	MOTA	3053	С	ASN	425	32.363	28.587	10.270	1.00	0.00		`3A4

ATOM	3054	o	ASN	425	33.092	28.033	9.449	1.00	0.00	3A4
ATOM	3055	N	ILE	426	32.734	28.773	11.570	1.00	0.00	3A4
ATOM	3056	CA	ILE	426	34.043	28.493	12.137	1.00	0.00	3A4
MOTA	3057	СВ	ILE	426	34.648	29.716	12.854	1.00	0.00	3A4 3A4
ATOM	3058		ILE	426	36.105 34.591	29.402 30.966	13.297 11.928	1.00	0.00	3A4
ATOM ATOM	3059 3060	CD	ILE	426 426	35.100	32.260	12.569	1.00	0.00	3A4
ATOM	3061	C	ILE	426	33.870	27.289	13.047	1.00	0.00	3A4
MOTA	3062	ō	ILE	426	34.107	26.155	12.633	1.00	0.00	3A4
MOTA	3063	N	ASP	427	33.447	27.532	14.315	1.00	0.00	3A4
ATOM	3064	CA	ASP	427	33.204	26.537	15.348	1.00	0.00	3A4
ATOM	3065	СВ	ASP	427	34.320	26.450	16.444 15.828	1.00	0.00	3A4 3A4
ATOM	3066	CG	ASP ASP	427 427	35.639 35.660	25.963 24.821	15.293	1.00	0.00	3A4
MOTA MOTA	3067 3068		ASP	427	36.643	26.722	15.888	1.00	0.00	3A4
ATOM	3069	C	ASP	427	31.841	26.813	15.973	1.00	0.00	3A4
ATOM	3070	0	ASP	427	31.098	25.842	16.103	1.00	0.00	3A4
ATOM	3071	N	PRO	428	31.390	28.043	16.369	1.00	0.00	3A4
MOTA	3072	CA	PRO	428	29.983	28.361	16.637	1.00	0.00	3A4
ATOM	3073	CD	PRO	428	32.272	29.141	16.778	1.00	0.00 0.00	3A4 3A4
ATOM	3074	CB	PRO	428 428	30.041 31.359	29.613 30.308	17.539 17.172	1.00	0.00	3A4
ATOM ATOM	3075 3076	CG C	PRO PRO	428	29.245	28.611	15.321	1.00	0.00	3A4
ATOM	3077	ŏ	PRO	428	29.471	29.640	14.687	1.00	0.00	3A4
ATOM .	3078	N	TYR	429	28.385	27.650	14.899	1.00	0.00	3A4
ATOM	3079	CA	TYR	429	27.755	27.649	13.596	1.00	0.00	3A4
MOTA	3080	CB	TYR	429	28.727	27.191	12.437	1.00	0.00	3A4
ATOM	3081	CG	TYR	429	29.325	25.786	12.428	1.00	0.00	3A4 3A4
ATOM	3082		TYR	429	29.871 29.371	25.334 24.901	11.208 13.532	1.00	0.00	3A4
ATOM ATOM	3083 3084		TYR TYR	429 429	30.418	24.050	11.078	1.00	0.00	3A4
ATOM	3085		TYR	429	29.917	23.615	13.410	1.00	0.00	3A4
ATOM	3086	CZ	TYR	429	30.437	23.186	12.181	1.00	0.00	3A4
ATOM	3087	ОН	TYR	429	30.972	21.885	12.055	1.00		3A4
ATOM	3088	С	TYR	429	26.500	26.805	13.683	1.00	0.00	3A4
ATOM	3089	0	TYR	429	25.984	26.542	14.769	1.00	0.00	3A4 3A4
ATOM	3090	N	ILE	430 . 430	26.004 24.912	26.339 25.392	12.499 12.301	1.00	0.00	374
MOTA MOTA	3091 3092	CA CB	ILE	430	23.953	25.845	11.196	1.00	0.00	3A4
ATOM	3093		ILE	430	23.323	27.171	11.680	1.00	0.00	3A4
ATOM	3094		ILE	430	24.623	26.004	9.800	1.00	0.00	3A4
ATOM	3095	CD	ILE	430	23.667	26.472	8.700	1.00	0.00	3A4
ATOM	3096	C	ILE	130	25.562	24.051	12.005	1.00	0.00	3A4 3A4
ATOM	3097	0	ILE	430	26.789 24.773	23.977 22.951	12.016 11.760	1.00	0.00 0.00	3A4
ATOM ATOM	3098 3099	N CA	TYR TYR	431 431	25.198	21.604	11.414	1.00	0.00	3A4
ATOM	3100	CB	TYR	431	26.437	21.470	10.410	1.00	0.00	3A4
ATOM	3101	CG	TYR	431	26.384	22.218	9.097	1.00	0.00	3A4
ATOM.	3102	CD1	TYR	431	25.749	21.647	7.983	1.00	0,00	3A4
ATOM	3103		TYR	431	27.142	23.393	8.894	1.00	0.00	3A4
ATOM	3104		TYR	431	25.834	22.246	6.714	1.00	0.00	3A4 3A4
ATOM	3105	CE2	TYR TYR	431 431	27.212 26.551	24.010 23.437	7.638 6.544	1.00	0.00	3A4
ATOM ATOM	3106 3107	OH	TYR	431	26.632	24.036	5.267	1.00	0.00	3A4
ATOM	3108	c c	TYR	431	25.647	20.889	12.688	1.00	0.00	3A4
ATOM	3109	0	TYR	431	26.635	21.285	13.303	1.00	0.00	3A4
MOTA	3110	N	THR	432	24.989	19.782	13.089	1.00	0.00	3A4
ATOM	3111	CA	THR	432	25.445	18.960	14.203	1.00	0.00	3A4 3A4
MOTA	3112	CB	THR	432	24.381 23.070	18.938 18.659	15.316 14.826	1.00	0.00	3A4
ATOM ATOM	3113 3114		THR	432 432	24.399	20.310	16.028	1.00	0.00	3A4
ATOM	3115	C	THR	432	25.810	17.558	13.781	1.00	0.00	3A4
ATOM	3116	ŏ	THR	432	25.565	16.648	14.576	1.00	0.00	3A4
MOTA	3117	N	PRO	433	26.389	17.234	12.610	1.00	0.00	3A4
MOTA	3118	CA	PRO	433	26.601	15.849	12.240	1.00	0.00	3A4
MOTA	3119	CD	PRO	433	27.173	18.101	11.724	1.00	0.00	3A4 3A4
ATOM	3120	CB	PRO	433 433	26.947 27.743	15.918 17.221	10.740 10.601	1.00	0.00	3A4
MOTA MOTA	3121 3122	CG C	PRO PRO	433	27.748	15.209	13.022	1.00	0.00	3A4
ATOM	3123	Õ	PRO	433	27.771	13.993	13.150	1.00	0.00	3A4
MOTA	3124	N	PHE -	434	28.673	16.013	13.587	1.00	0.00	3A4
ATOM	3125	CA	PHE	434	29.782	15.548	14.382	1.00	0.00	3A4

ATOM	3126	СВ	PHE	434	31.108	16.257	13.997	1.00	0.00	3A4
ATOM	3127	CG	PHE	434	31.591	15.810	12.639	1.00	0.00	3A4
ATOM	3128	CD1	PHE	434	31.353	16.451	11.514	1.00	0.00	3A4
MOTA	3129	CD2		434	32.354	14.754	12.363	1.00	0.00	3A4 3A4
ATOM	3130	CEI		434	31.813 32.860	16.203 14.287	10.200 11.129	1.00	0.00	3A4
ATOM	3131 3132	CE2	PHE	434 434	32.592	15.066	10.009	1.00	0.00	3A4
ATOM ATOM	3132	C	PHE	434	29.528	15.802	15.833	1.00	0.00	3A4
ATOM	3134	ŏ	PHE	434	30.427	15.663	16.655	1.00	0.00	3A4
ATOM	3135	N	GLY	435	28.291	16.210	16.191	1.00	0.00	3A4
ATOM	3136	CA	GLY	435	27.923	16.495	17.561	1.00	0.00	3A4 3A4
MOTA	3137	C	GLY	435	28.209 28.305	17.917 18.719	17.875 16.943	1.00	0.00	3A4
ATOM	3138 3139	о И	GLY SER	435 436	28.348	18.248	19.183	1.00	0.00	3A4
ATOM ATOM	3140	CA	SER	436	28.384	19.623	19.578	1.00	0.00	3A4
ATOM	3141	CB	SER	436	26.947	20.258	19.543	1.00	0.00	3A4
ATOM	3142	OG	SER	436	26.948	21.683	19.489	1.00	0.00	3A4
MOTA	3143	C	SER	436	29.197	19.916	20.769	1.00 1.00	0.00	3A4 3A4
ATOM	3144	0	SER	436 437	30.134 28.951	20.642 19.486	21.973	1.00	0.00	3A4
ATOM ATOM	3145 3146	N CA	GLY	437	29.675	19.961	23.144	1.00	0.00	3A4
ATOM	3147	c c	GLY	437	31.130	19.558	23.314	1.00	0.00	3A4
MOTA	3148	0	GLY	437	31.959	19.487	22.402	1.00	0.00	3A4
MOTA	3149	N	PRO	438	31.502	19.228	24.529	1.00	0.00	3A4 3A4
ATOM	3150	CA	PRO	438	32.875 30.927	18.727 19.742	24.776 25.770	1.00	0.00	3A4
ATOM ATOM	3151 3152	CD CB	PRO	438 - 438	33.100	18.880	26.266	1.00	0.00	3A4
ATOM	3153	CG	PRO	438	31.706	19.063	26.880	1.00	0.00	· 3A4
ATOM	3154	C	PRO	438	33.099	17.295	24.317	1.00	0.00	3A4
ATOM	3155	0	PRO	438	34.230	16.824	24.348	1.00	0.00	3A4 3A4
MOTA	3156	N	ARG	439	32.033	16.608 15.264	23.850 23.366	1.00	0.00	3A4
MOTA	3157	CA CB	ARG ARG	439 439	32.068 30.905	14.467	23.961	1.00	0.00	3A4
ATOM ATOM	3158 3159	CG	ARG	439	30.793	14.766	25.461	1.00	0.00	3A4
ATOM	3160	CD	ARG	439	30.197	13.690	26.366	1.00	0.00	3A4
ATOM	3161	NE	ARG	439	30.391	14.136	27.786	1.00	0.00	3A4 3A4
MOTA	3162	CZ	ARG	439	30.091	13.354	28.866 30.116	1.00	0.00	3A4
MOTA	3163		ARG	439 439	30.342 29.553	13.836 12.109	28.713	1.00	0.00	3A4
ATOM ATOM	3164 3165	C	ARG	439	31.980	15.221	21.890	1.00	0.00	3A4
ATOM	3166	ō	ARG	439	31.776	14.165	21.309	1.00	0.00	3A4
ATOM	3167	N	ASN	440	32.201	16.364	21.200	1.00	0.00	3A4
MOTA	3168	CA	ASN	440	32.204	16.474	19.756	1.00	0.00	3A4 3A4
MOTA	3169	CB CG	ASN	440 440	32.625 32.279	17.886 18.329	19.354 17.901	1.00	0.00	3A4
ATOM ATOM	3170 3171		ASN ASN	440	32.746	17.778	16.907	1.00	0.00	3A4
ATOM	3172		ASN	440	31.452	19.401	17.765	1.00	0.00	3A4
ATOM	3173	С	ASN	440	33.216	15.539	19.171	1.00	0.00	3A4
ATOM	3174	0	ASN	440.	34.241	15.285	19.807	1.00	0.00	3A4 3A4
ATOM	3175	N CA	CYS	441 441	32.950 33.782	14.993 14.009	17.974 17.328	1.00 1.00	0.00	3A4
ATOM ATOM	3176 3177	CB	CYS	441	33.288	13.772	15.899	1.00	0.00	3A4
ATOM	3178	SG	CYS	441	34.028	12.338	15.029	1.00	0.00	3A4
MOTA	3179	С	CYS	441	35.241	14.414	17.264		0.00	3A4
ATOM	3180	0	CYS	441	35.564	15.528	16.866	1.00	0.00	3A4 3A4
ATOM	3181	N CA	ILE	442 442	-36.131 37.556	13.531 13.799	17.746 17.790	1.00	0.00	3A4
ATOM ATOM	3182 3183	CB	ILE	442	38.223	12.944	18.848	1.00	0.00	3A4
ATOM	3184		ILE	442	38.388	11.476	18.448	1.00	0.00	3A4
MOTA	3185	CG1	ILE	442	39.528	13.570	19.391	1.00	0.00	3A4
MOTA	3186	CD	ILE	442	39.336	14.819	20.250	1.00	0.00	3A4 3A4
ATOM	3187	C	ILE	442 442	38.181 39.180	13.605 14.220	16.408 16.048	1.00	0.00	3A4
ATOM ATOM	3188 3189	0 N	ILE	442	37.524	12.758	15.590		0.00	3A4
ATOM	3190	CA	GLY	443	37.942	12.408	14.266	1.00	0.00	3A4
ATOM	3191	С	GLY	443	37.399	13.252	13.158		0.00	3A4
MOTA	3192	0	GLY	443	37.591	12.902	12.001		0.00	3A4 3A4
MOTA	3193	N	MET	444 444	36.732 36.082	14.396 15.266	13.456 12.493			3A4
ATOM ATOM	3194 3195	CA CB	MET MET	444	35.408	16.458	13.192			3A4
ATOM	3196	CG	MET	444	36.294	17.310	14.126	_	0.00	3A4
ATOM	3197	SD	MET	444	35.375	18.583	15.041	1.00	0.00	3A4

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MOTA	3198	CE	MET	444		36.695	18.911	16.244	1.00	0.00	3A4
MOTA	3199	С	MET	444	•	36.968	15.807	11.395	1.00	0.00	3A4
ATOM	3200	0	MET	444		36.570	15.844	10.236	1.00	0.00	3A4
ATOM	3201	N	ARG	445		38.230	16.170	11.727	1.00	0.00	3A4 3A4
ATOM ATOM	3202 3203	CA CB	ARG ARG	445 445		39.211 40.435	16.708 17.321	10.801 11.549	1.00	0.00	3A4
ATOM	3204	CG	ARG	445		40.058	18.332	12.647	1.00	0.00	3A4
ATOM	3205	CD	ARG	445		39.223	19.529	12.155	1.00	0.00	3A4
ATOM	3206	NE	ARG	445		38.880	20.389	13.341	1.00	0.00	3A4
ATOM	3207	CZ	ARG	445		37.901	21.351	13.313	1.00	0.00	3A4
MOTA	3208	NH1		445		37.643	22.071	14.443	1.00	0.00	3A4 3A4
ATOM	3209	NH2 C	ARG	445 445		37.171 39.695	21.600 15.651	12.186 9.828	1.00	0.00	3A4
ATOM ATOM	3210 3211	ò	ARG	445		39.790	15.886	8.628	1.00	0.00	3A4
ATOM	3212	N	PHE	446		39.920	14.418	10.335	1.00	0.00	3A4
MOTA	3213	CA	PHE	446		40.293	13.256	9.549	1.00	0.00	3A4
MOTA	3214	СВ	PHE	446		40.683	12.116	10.501	1.00	0.00	3A4
ATOM	3215	CG	PHE	446		41.549	11.008	9.982	1.00	0.00	3A4 3A4
ATOM	3216	CD1		446 446		42.800 41.248	11.292 9.684	9.403 10.350	1.00	0.00	3A4
ATOM ATOM	3217 3218	CD2		446		43.749	10.278	9.241	1.00	0.00	3A4
ATOM	3219	CE2		446		42.210	8.678	10.222	1.00	0.00	3A4
ATOM	3220	CZ	PHE	446		43.469	8.983	9.689	1.00	0.00	3A4
ATOM	3221	С	PHE	446		39.172	12.804	8.647	1.00	0.00	3A4
ATOM	3222	0	PHE	446		39.384	12.508	7.480	1.00	0.00	3A4
ATOM	3223	N	ALA	447		37.921	12.812	9.148 8.393	1.00	0.00	3A4 3A4
ATOM ATOM	3224 3225	CA CB	ALA ALA	447 447		36.738 35.499	12.472 12.464	9.272	1.00	0.00	3A4
ATOM	3226	C	ALA	447		36.489	13.392	7.228		0.00	3A4
ATOM	3227	ō	ALA	447		36.216	12.950	6.120	1.00	0.00	3A4
ATOM	3228	N	LEU	448		36.656	14.715	7.427	1.00	0.00	3A4
ATOM	3229	CA	LEU	448		36.469	15.704	6.386	1.00	0.00	3A4
ATOM	3230	CB	LEU	448		36.399 35.089	17.124	6.962 7.731	1.00	0.00	3A4 3A4
ATOM ATOM	3231 3232	CG CD1	LEU	448 448		35.223	17.408 18.721	8.515	1.00	0.00	3A4
ATOM	3233	CD2		448		33.842	17.445	6.826	1.00	0.00	3A4
ATOM	3234	c	LEU	448		37.561	15.661	5.351	1.00	0.00	3A4
ATOM	3235	0	LEU	448		37.299	15.865	4.175	1.00	0.00	3A4
ATOM	3236	N .	MET	449		38.806	15.319	5.746	1.00	0.00	3A4
ATOM	3237	CA	MET	449		39.935 41.269	15.178 15.033	4.853 5.617	1.00	0.00	3A4 3A4
ATOM ATOM	3238 3239	CB CG	MET MET	449 449		41.269	16.358	6.130	1.00	0.00	3A4
ATOM	3240	SD	MET	449		43.382	16.135	7.075	1.00	0.00	3A4
ATOM	3241	CE	MET	449		43.701	17.904	7.332	1.00	0.00	3A4
ATOM	3242	C	MET	449		39.772	13.984	3.951	1.00	0.00	3A4
ATOM	3243	0	MET	449		39.956	14.095	2.746	1.00	0.00	3A4 3A4
ATOM	3244	N CA	ASN	450 450		39.332 39.098	12.829 11.625	4.502 3.740	1.00	0.00	3A4
MOTA MOTA	3245 3246	CB	ASN ASN	450		38.915	10.385	4.623	1.00	0.00	3A4
ATOM	3247	CG	ASN	450		37.685	10.130	5.531	1.00	0.00	3A4
ATOM	3248	OD1	ASN	450		36.512	10.268	5.191	1.00	0.00	3A4
MOTA	3249	ND2		450		37.990	9.606	6.751	1.00	0.00	3A4
MOTA	3250	С	ASN	450		37.976	11.740	2.750	1.00	0.00	3A4 3A4
ATOM	3251 3252	N.	ASN MET	450 451		38.095 36.874	11.281 12.422	1.623 3.129	1.00	0.00	3A4
ATOM ATOM	3253	CA	MET	451		35.744	12.687	2.267	1.00	0.00	3A4
ATOM	3254	СВ	MET	451		34.596	13.445	3.021	1.00	0.00	3A4
ATOM	3255	CG	MET	451		33.788	12.610	4.010	1.00	0.00	3A4
MOTA	3256	SD	MET	451		32.502	13.565	4.863	1.00	0.00	3A4
MOTA	3257	CE	MET	451		33.061	13.383	6.570	1.00	0.00	3A4 3A4
ATOM	3258	C	MET	451 451		36.081 35.746	13.580 13.314	1.106 -0.041	1.00	0.00	3A4
MOTA MOTA	3259 3260	N O	MET Lys	451 452		36.821	14.667	1.389	1.00	0.00	3A4
ATOM	3261	CA	LYS	452		37.237	15.652	0.424	1.00	0.00	3A4
ATOM	3262	СВ	LYS	452		37.854	16.860	1.154	1.00	0.00	3A4
ATOM	3263	CG	LYS	452		37.750	18.227	0.470	1.00	0.00	3A4
MOTA	3264	CD	LYS	452		38.346	19.380	1.301	1.00	0.00	3A4 3A4
ATOM	3265 3266	CE NZ	LYS	452 452		38.006 36.543	19.391 19.337	2.808 3.053	1.00	0.00	3A4
ATOM ATOM	3266 3267	NZ C	LYS LYS	452 452		38.228	15.110	-0.572	1.00	0.00	3A4
ATOM	3268	Ö	LYS	452		38.108	15.335	-1.769	1.00	0.00	3A4
ATOM	3269	N	LEU	453		39.207	14.309	-0.102	1.00	0.00	3A4

ATOM	3270	CA	LEU	453	40.212	13.676	-0.927	1.00	0.00	3A4
ATOM	3271	СВ	LEU	453	41.342	13.071	-0.061	1.00	0.00	3A4
MOTA	3272	CG	LEU	453	42.298	14.219	0.403	1.00	0.00	3A4
ATOM	3273	CD1	LEU	453	43.187	13.854	1.595	1.00	0.00	3A4
MOTA	3274	CD2	LEU	453	43.191	14.764	-0.734	1.00	0.00	3A4
MOTA	3275	С	LEU	453	39.621	12.644	-1.845	1.00	0.00	3A4
MOTA	3276	0	LEU	453	39.939	12.613	-3.026	1.00	0.00	3A4
ATOM	3277	N	λLA	454	38.662	11.829	-1.353	1.00	0.00	3A4
MOTA	3278	CA	ALA	454	37.935	10.847	-2.131	1.00	0.00	3A4
MOTA	3279	СВ	ALA	454	37.013	9.992	-1.240	1.00	0.00	3A4
ATOM	3280	С	ALA	454	37.093	11.464	-3.225	1.00	0.00	3A4
ATOM	3281	0	ALA	454	37.181	11.055	-4.371	1.00	0.00	3A4
ATOM	3282	N	LEU	455	36.307	12.514	-2.904	1.00	0.00	3A4
MOTA	3283	CA	LEU	455	35.457	13.201	-3.852	1.00	0.00	3A4
MOTA	3284	СВ	LEU	455	34.480	14.157	-3.157	1.00	0.00	3A4
MOTA	3285	CG	LEU	455	33.366	13.559	-2.303	1.00	0.00	3A4
ATOM	3286	CD1	LEU	455	32.576	14.761	-1.760	1.00	0.00	3A4
MOTA	3287	CD2	LEU	455	32.474	12.556	-3.064	1.00	0.00	3A4
MOTA	3288	C	LEU	455	36.203	14.018	-4.886	1.00	0.00	3A4
MOTA	3289	0	LEU	455	35.736	14.147	-6.009	1.00	0.00	3A4
MOTA	3290	N	ILE	456	37.412	14.540	-4.555	1.00	0.00	3A4
ATOM	3291	CA	ILE	456	38.284	15.264	-5.474	1.00	0.00	3A4
MOTA	3292	CB	ILE	456	39.413	16.061	-4.749	1.00	0.00	3A4
MOTA	3293		ILE	456	40.832	16.074	-5.412	1.00	0.00	3A4
MOTA	3294		ILE	456	39.003	17.537	-4.565	1.00	0.00	3A4
MOTA	3295	CD	ILE	456	38.041	17.823	-3.423	1.00	0.00	3A4
ATOM	3296	С	ILE	456	38.894	14.318	-6.496	1.00	0.00	3A4
ATOM	3297	0	IFE	456	39.099	14.677	-7.647	1.00	0.00	3A4
ATOM	3298	N	ARG	457	39.181	13.066	-6.083	1.00	0.00	3A4
ATOM	3299	CA	ARG	457	39.859	12.081	-6.895	1.00	0.00	3A4
ATOM	3300	СВ	ARG	457	40.758	11.186	-6.025	1.00	0.00	3A4 3A4
MOTA	3301	CG	ARG	457	41.905	12.005	-5.430	1.00	0.00	
ATOM	3302	CD	ARG	457	42.735	11.300	-4.341 -3.632	1.00	0.00	3A4 3A4
ATOM	3303	NE	ARG	457	43.559	12.343		1.00	0.00	3A4
ATOM	3304	CZ	ARG	457	44.624	12.985	-4.211 -3.601	1.00	0.00	3A4
ATOM	3305		ARG	457	45.148 45.174	14.087 12.558	-5.385	1.00	0.00	3A4
ATOM ATOM	3306 3307		ARG ARG	457 457	38.924	11.235	-7.722	1.00	0.00	3A4
ATOM	3308	C O	ARG	457	39.246	10.873	-8.848	1.00	0.00	3A4
ATOM	3309	N	VAL	458	37.713	10.918	-7.207	1.00	0.00	3A4
ATOM	3310	CA	VAL	458	36.711	10.092	-7.872	1.00	0.00	3A4
ATOM	3311	СВ	VAL	458	35.631	9.662	-6.887	1.00	0.00	3A4
ATOM	3312	CG1	VAL	458	34.290	9.133	-7.471	1.00	0.00	3A4
ATOM	3313	CG2		458	36.253	8.556	-6.006	1.00	0.00	3A4
ATOM	3314	c	VAL	458	36.101	10.798	-9.063	1.00	0.00	3A4
ATOM	3315	ō.	VAL	458	36.040		-10.146	1.00	0.00	3A4
ATOM	3316	N	LEU	459	35.685	12.071	-8.900	1.00	0.00	3A4
ATOM	3317	CA	LEU	459	34.979	12.841	-9.906	1.00	0.00	3A4
ATOM	3318	СВ	LEU	459	34.354	14.096	-9.255	1.00	0.00	3A4
ATOM	3319	CG	LEU	459	33.225	13.778	-8.265	1.00	0.00	3A4
MOTA	3320		LEU	459	32.786	15.037	-7.500	1.00	0.00	3A4
ATOM	3321	CD2	LEU	459	32.041	13.132	-8.991	1.00	0.00	3A4
MOTA	3322	С	LEU	459	35.826	13.309	-11.060	1.00	0.00	3A4
MOTA	3323	0	LEU	459	35.319	13.601	-12.136	1.00	0.00	3A4
MOTA	3324	N	GLN	460	37.158	13.371	-10.874	1.00	0.00	3A4
MOTA	3325	CA	GLN	460	38.070	13.748	-11.927	1.00	0.00	3A4
MOTA	3326	CB	GLN	460	39.373	14.365	-11.376	1.00	0.00	3A4
MOTA	3327	CG	GLN	460	39.106	15.740	-10.736	1.00	0.00	3A4
MOTA	3328	CD	GLN	460	40.408	16.286	-10.160	1.00	0.00	3A4
ATOM	3329	OE1	GLN	460	41.430	15.608	-10.237	1.00	0.00	3A4
ATOM	3330	NE2	GLN	460	40.380	17.515	-9.575	1.00	0.00	3A4
MOTA	3331	С	GLN	460	38.365		-12.815	1.00	0.00	3A4
MOTA	3332	0	GLN	460	38.683		-13.990	1.00	0.00	3A4
MOTA	3333	N	ASN	461	38.258		-12.266	1.00	0.00	3A4
ATOM	3334	CA	ASN	461	38.598		-12.957	1.00	0.00	3A4
ATOM	3335	СВ	ASN	461	39.328		-12.018	1.00	0.00	3A4
ATOM	3336	CG	ASN	461	40.725		-11.730	1.00	0.00	3A4
ATOM	3337	OD1		461	41.364		-12.617	1.00	0.00	3A4
ATOM	3338	ND2		461	41.239		-10.482	1.00	0.00	3A4
ATOM	3339	С	ASN	461	37.402		-13.562	1.00	0.00	3A4
MOTA	3340	0	ASN	461	37.588		-14.451	1.00	0.00	3A4
ATOM	3341	N	PHE	462	36.167	9.725	-13.107	1.00	0.00	3A4

ATOM	3342	CA	PHE	462	34.983	8.975 -13.533	1.00	0.00	3A4
ATOM	3343	СВ	PHE	462	34.346	8.159 -12.354	1.00	0.00	3A4
ATOM.	3344	CG	PHE	462	35.274	7.073 -11.873	1.00	0.00	3A4 3A4
ATOM	3345	CD1		462 462	35.686 35.718	6.051 -12.745 7.025 -10.540	1.00	0.00 0.00	3A4
MOTA MOTA	3346 3347	CD2 CE1		462	36.530	5.021 -12.307	1.00	0.00	3A4
ATOM	3348	CE2		462	36.561	6.001 -10.089	1.00	0.00	3A4
ATOM	3349	CZ	PHE	462	36.972	5.002 -10.978	1.00	0.00	3A4
ATOM	3350	С	PHE	462	33.836	9.848 -14.135	1.00	0.00	3A4
ATOM .	3351	0	PHE	462	33.734	11.037 -13.828	1.00	0.00 0.00	3A4 3A4
ATOM	3352	N	SER	463 463	32.784 31.446	9.198 -15.007 9.622 -15.542	1.00	0.00	3A4
ATOM ATOM	3353 3354	CA CB	SER SER	463	31.400	9.685 -17.094	1.00	0.00	3A4
ATOM	3355	OG	SER	463	32.293	10.684 -17.565	1.00	0.00	3A4
ATOM	3356	С	SER	463	30.513	8.581 -15.014	1.00	0.00	3A4
ATOM	3357	0	SER	463	30.243	7.578 -15.673	1.00	0.00	3A4
ATOM	3358	N	PHE	464	30.012	8.774 -13.767	1.00	0.00 0.00	3A4 3A4
ATOM	3359	CA	PHE	464 464	29.251 29.689	7.754 -13.078 7.483 -11.603	1.00	0.00	3A4
ATOM ATOM	3360 3361	CB CG	PHE PHE	464	29.600	8.582 -10.565	1.00	0.00	3A4
ATOM	3362	CD1		464	30.780	9.102 ~9.999	1.00	0.00	3A4
ATOM	3363	CD2		464	28.364	8.952 -9.990	1.00	0.00	3A4
ATOM	3364		PHE	464	30.727	9.958 -8.891	1.00	0.00	3A4 3A4
ATOM	3365		PHE	464	28.310 29.493	9.832 -8.899 10.333 -8.347	1.00	0.00 0.00	3A4
ATOM ATOM	3366 3367	CZ C	PHE	464 464	27.768	7.948 -13.199	1.00	0.00	3A4
ATOM	3368	ŏ	PHE	464	27.238	9.056 -13.175	1.00	0.00	3A4
ATOM	3369	N	LYS	465	27.076	6.801 -13.331	1.00	0.00	3A4
ATOM	3370	CA	LYS	465	25.646	6.719 -13.439	1.00	0.00	3A4
ATOM	3371	CB	LYS	465	25.197	6.398 -14.891	1.00	0.00	3A4 3A4
ATOM	3372	CG	LYS	465 465	25.553 25.067	7.484 -15.915 7.162 -17.333	1.00	0.00	3A4
ATOM ATOM	3373 3374	CD CE	LYS LYS	465	25.438	8.228 -18.374	1.00	0.00	3A4
ATOM	3375	NZ	LYS	465	26.910	8.360 -18.512	1.00	0.00	3A4
ATOM	3376	С	LYS	465	25.212	5.614 -12.507	1.00	0.00	3A4
MOTA	3377	0	LYS	465	25.982	4.688 -12.254	1.00	0.00	- 3A4 3A4
MOTA	3378	N	PRO	466	23.983 23.422	5.622 -11.985 4.511 -11.249	1.00	0.00	3A4
ATOM ATOM	3379 3380	CA CD	PRO PRO	466 466	23.422	6.783 -11.993	1.00	0.00	3A4
ATOM	3381	СВ	PRO	466	22.300	5.151 -10.405	1.00	0.00	3A4
ATOM	3382	CG	PRO	466	21.827	6.358 -11.228	1.00	0.00	3A4
ATOM	3383	С	PRO	466	22.906	3.470 -12.228	1.00	0.00	3A4
ATOM	3384	0	PRO	466	22.333	3.808 -13.264 2.179 -11.890	1.00	0.00	3A4 3A4
ATOM	3385 3386	N CA	CYS	467 467	23.088 22.624	1.049 -12.667	1.00	0.00	3A4
ATOM ATOM	3387	CB	CYS	467	23.617	-0.143 -12.501	1.00	0.00	3A4
ATOM	3388	SG	CYS	467	23.434	-1.534 -13.674	1.00	0.00	3A4
ATOM	3389	С		467	21.212	0.659 -12.220	1.00	0.00	3A4
ATOM .	3390	0	CYS	467	20,555	-0.179 -12.834 1.325 -11.130	1.00	0.00	3A4 3A4
MOTA MOTA	3391 3392	N CA	LYS LYS	468 468	20.726 19.389	1.282 -10.573	1.00	0.00	3A4
ATOM	3393	СВ	LYS	468	19.406	1.410 -9.027	1.00	0.00	3A4
ATOM	3394	CG	LYS	468	20.290	0.367 -8.339	1.00	0.00	3A4
MOTA	3395	CD	LYS	468	20.136	0.413 -6.821			3A4
ATOM	3396	CE	LYS	468	21.077	-0.534 -6.078 -0.485 -4.626	1.00	0.00	3A4 3A4
MOTA MOTA	3397 3398	NZ C	LYS LYS	468 468	20.807 18.586	-0.485 -4.626 2.429 -11.148	1.00	0.00	3A4
ATOM	3399	ŏ	LYS	468	19.145	3.450 -11.548	1.00	0.00	3A4
ATOM	3400	N	GLU	469	17.238	2.263 -11.203	1.00	0.00	3A4
ATOM	3401	CA	GLU	469	16.301	3.177 -11.832	1.00	0.00	3A4
ATOM	3402	CB	GLU	469	15.428	2.446 -12.905	1.00	0.00	3A4 3A4
ATOM	3403	CG	GLU	469 469	16.234 17.104	1.719 -14.000 2.712 -14.780	1.00	0.00	3A4
MOTA MOTA	3404 3405	CD OE1	GLU	469	16.530	3.642 -15.407	1.00	0.00	3A4
ATOM	3406		GLU	469	18.355	2.551 -14.761	1.00	0.00	3A4
ATOM	3407	С	GLU	469	15.433	3.792 -10.753	1.00	0.00	3A4
MOTA	3408	0	GLU	469	15.841	3.909 -9.598	1.00	0.00	3A4 3A4
ATOM	3409	N	THR	470 470	14.183 13.125	4.182 -11.133 4.722 -10.289	1.00		3A4 3A4
MOTA MOTA	3410 3411	CA CB	THR THR	470 470	12.400	5.877 -10.998	1.00		3A4
ATOM	3412		THR	470	11.519	6.597 -10.138	1.00		3A4
ATOM	3413		THR	470	11.657	5.427 -12.286	1.00	0.00	3A4

ATOM	3414	С	THR	470	12.198	3.578	-9.882	1.00	0.00	3A4
ATOM	3415	ŏ	THR	470	11.456	3.677	-8.906	1.00	0.00	3A4
ATOM	3416	N	GLN	471	12.279	2.447 -	10.640	1.00	0.00	3A4
ATOM	3417	CA	GLN	471	11.670	1.158 -	10.385	1.00	0.00	3A4
ATOM	3418	CB	GLN	471	10.997	0.559 -		1.00	0.00	3A4
ATOM	3419	CG	GLN	471	11.811	0.665 -	_	1.00	0.00	3A4 3A4
MOTA	3420	CD	GLN	471	10.976	0.103 -		1.00	0.00	3A4
MOTA	3421		GLN	471	10.763	-1.106 - 0.985 -		1.00	0.00	3A4
ATOM	3422	NE2		471 471	10.489 12.773	0.985	-9.839	1.00	0.00	3A4
MOTA	3423	С О	GLN GLN	471	13.605	-0.249		1.00	0.00	3A4
ATOM ATOM	3424 3425	N	ILE	472	12.809	0.178	-8.475	1.00	0.00	3A4
ATOM	3426	CA	ILE	472	13.847	-0.369	-7.600	1.00	0.00	3A4
ATOM	3427	СВ	ILE	472	14.451	-1.737	-7.993	1.00	0.00	3A4
ATOM	3428	CG2	ILE	472	15.447	-2.232	-6.907	1.00	0.00	3A4
MOTA	3429	CGI	ILE	472	13.359	-2.820	-8.240	1.00	0.00	3A4
ATOM	3430	CD	ILE	472	12.440	-3.129	-7.050	1.00	0.00 0.00	3A4 3A4
ATOM	3431	С	ILE	472	14.926	0.710	-7.400 -8.188	1.00	0.00	3A4
ATOM	3432	0	ILE	472	15.870 14.837	0.760 1.594	-6.373	1.00	0.00	3A4
MOTA	3433	N	PRO	473 473	15.865	2.553	-5.978	1.00	0.00	3A4
MOTA	3434 3435	CA CD	PRO PRO	473	13.607	1.778	-5.600	1.00	0.00	3A4
ATOM ATOM	3436	CB	PRO	473	15.047	3.657	-5.263	1.00	0.00	3A4
ATOM	3437	CG	PRO	473	13.885	2.910	-4.607	1.00	0.00	3A4
ATOM	3438	c	PRO	473	16.926	1.936	-5.117	1.00	0.00	3A4
ATOM	3439	0	PRO	473	17.147	0.726	-5.098	1.00	0.00	3A4
ATOM	3440	N	LEU	474	17.606	2.821	-4.384	1.00	0.00	3A4
MOTA	3441	CA	LEU	474	18.692	2.518	-3.506	1.00	0.00	3A4 3A4
ATOM	3442	CB	LEU	474	19.658	3.718	-3.467 -2.623	1.00	0.00 0.00	3A4
ATOM	3443	CG	LEU	474	20.935 22.187	3.548 3.637	-3.503	1.00	0.00	3A4
MOTA	3444		LEU	474 474	20.962	4.569	-1.472	1.00	0.00	3A4
ATOM ATOM	3445 3446	CDZ	LEU	474	18.157	2.198	-2.136	1.00	0.00	3A4
ATOM	3447	ŏ	LEU	474	17.397	2.966	-1.547	1.00	0.00	3A4
ATOM	3448	N	LYS	475	18.561	1.016	-1.612	1.00	0.00	3A4
ATOM	3449	CA	LYS	475	18.133	0.502	-0.330	1.00	0.00	3A4
MOTA	3450	CB	LYS	475	18.199	-1.049	-0.249	1.00	0.00	3A4 3A4
ATOM	3451	CG	LYS	475	17.520	-1.656	0.999	1.00	0.00 0.00	3A4
MOTA	3452	CD	LYS	475	17.579	-3.189 -3.776	1.074	1.00	0.00	3A4
ATOM	3453	CE	LYS	475	18.981 19.572	-3.776	2.580	1.00	0.00	3A4
ATOM	3454	NZ C	LYS LYS	475 475	18.961	1.086	0.775	1.00	0.00	3A4
ATOM ATOM	3455 3456	ò	LYS	475	20.173	0.909	0.825	1.00	0.00	3A4
ATOM	3457	N	LEU	476	18.276	1.798	1.695	1.00	0.00	3A4
ATOM	3458	CA	LEU	476	18.860	2.419	2.855	1.00	0.00	3A4
ATOM	3459	CB ·	LEU	476	18.422	3.903	3.070	1.00	0.00	3A4
MOTA	3460		·LEU	476	16.930	4.243	3.360	1.00	0.00	-3A4 3A4
MOTA	3461		LEU	476	16.813	5.725	3.764 2.201	1.00	0.00	3A4
MOTA	3462		LEU	476 .	15.956	3.930 1.579	4.038	1.00	0.00	3A4
ATOM	3463	C	LEU	476 476	18.580 17.524	0.970	4.149	1.00	0.00	3A4
ATOM ATOM	3464 3465	N.	SER	477	19.543	1.495	4.973	1.00	0.00	_ 3A4
ATOM	3466	CA	SER	477	19.480	0.545	6.040	1.00	0.00	3A4
ATOM	3467	СВ	SER	477	20.807	-0.220	6.343	1.00	0.00	3A4
MOTA	3468	OG	SER	477	20.584	-1.554	6.795	1.00	0.00	3A4
ATOM	3469	С	SER		18.826	1.150	7.228	1.00		3A4 3A4
MOTA	3470	0	SER		18.936	2.334	7.525	1.00		3A4
MOTA	3471	N	LEU	478	18.068	0.282 0.588	7.917 9.132	1.00		3A4
MOTA	3472	CA	LEU	478	17.386 16.072	-0.245	9.288	1.00		3A4
ATOM	3473	CB	LEU	478 478	15.314	-0.208	10.653	1.00		3A4
ATOM ATOM	3474 3475	CG CD1	LEU LEU		14.954	1.206	11.152	1.00		3A4
ATOM	3476		LEU		14.057	-1.098	10.607	1.00	0.00	3A4
ATOM	3477	C	LEU		18.338	0.280		1.00		3A4
ATOM	3478	0	LEU		18.566	-0.855	10.665	1.00		3A4
ATOM	3479	N	GLY		18.982	1.308		1.00		3A4 3A4
MOTA	3480	CA	GLY		19.983	1.119		1.00		3A4
ATOM	3481	C	GLY		19.558	1.665 0.936		1.00		3A4
MOTA	3482	0	GLY		19.405 19.416	2.996				3A4
ATOM	3483	N CA	GLY GLY		19.205					3A4
ATOM ATOM	3484 3485	CA	GLY		20.442					3A4
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ATOM	3486	0	GLY	480	20.430	5.574	14.961	1.00	0.00	3A4
ATOM	3487	N	LEU	481	21.566	3.643	15.196	1.00	0.00	3A4
ATOM	3488	CA	LEU	481	22.833	4.218	15.597	1.00	0.00	3A4
ATOM	3489	СВ	LEU	481	23.634	3.303	16.586	1.00	0.00 0.00	3A4 3A4
MOTA	3490	CG	LEU	481	23.971 25.057	1.830 1.273	16.194 17.135	1.00	0.00	3A4
ATOM	3491 3492	CD1 CD2		481 481	22.767	0.861	16.168	1.00	0.00	3A4
ATOM ATOM	3493	CD2	LEU	481	23.664	4.637	14.398	1.00	0.00	3A4
ATOM	3494	<u>o</u> .	LEU	481	24.121	5.774	14.349	1.00	0.00	3A4
ATOM	3495	N	LEU	482	23.838	3.733	13.398	1.00	0.00	3A4
ATOM	3496	CA	LEU	482	24.486	3.984	12.124	1.00	0.00	3A4 3A4
MOTA	3497	СВ	LEU	482	25.613	2.951	11.765 12.517	1.00	0.00	3A4
MOTA	3498	CG	LEU	482 482	26.965 27.722	3.067 4.365	12.317	1.00	0.00	3A4
ATOM ATOM	3499 3500	CD1 CD2		482	26.897	2.808	14.028	1.00	0.00	3A4
ATOM	3501	C	LEU	482	23.378	3.835	11.115	1.00	0.00	3A4
ATOM	3502	ō	LEU	482	22.784	2.766	11.044	1.00	0.00	3A4
ATOM	3503	N	GLN	483	23.090	4.887	10.291	1.00	0.00	3A4
ATOM	3504	CA	GLN	483	22.131	4.849	9.194	1.00	0.00	3A4
ATOM	3505	СВ	GLN	483	21.199	6.105	9.194 10.449	1.00	0.00	3A4 3A4
ATOM	3506	CG	GLN	483 483	20.316 19.134	6.274 5.295	10.449	1.00	0.00	3A4
ATOM ATOM	3507 3508	CD	GLN GLN	483	18.982	4.423	9.605	1.00	0.00	3A4
ATOM	3509		GLN	483	18.236	5.459	11.467	1.00	0.00	3A4
ATOM	3510	c	GLN	483	22.916	4.815	7.900	1.00	0.00	3A4
ATOM	3511	0	GLN	483	23.541	5.820	7.606	1.00	0.00	3A4
ATOM	3512	N	PRO	484	22.951	3.748	7.093	1.00	0.00	3A4 3A4
MOTA	3513	CA	PRO	484	23.817	3.721	5.925 7.687	1.00	0.00	3A4
ATOM	3514	CD	PRO	484 484	22.874 24.769	2.409 2.558	6.262	1.00	0.00	3A4
ATOM ATOM	3515 3516	CB CG	PRO PRO	484	23.861	1.520	6.915	1.00	0.00	3A4
ATOM	3517	c	PRO	484	23.035	3.412	4.673	1.00	0.00	3A4
ATOM	3518	0	PRO	484	21.816	3.307	4.680	1.00	0.00	3A4
ATOM	3519	N	GLU	485	23.773	3.212	3.562	1.00	0.00	3A4
MOTA	3520	CA	GLU	485	23.248	2.558	2.383	1.00	0.00	3A4 3A4
ATOM	3521	СВ	GLU	485	23.098 24.327	3.493 4.316	1.177 0.781	1.00 1.00	0.00	3A4
ATOM	3522 3523	CG CD	GTA GTA	485 485	24.829	3.771	-0.540	1.00	0.00	3A4
ATOM ATOM	3524		GLU	485	24.837	4.541	-1.536	1.00	0.00	3A4
ATOM	3525		GLU	485	25.209	2.571	-0.567	1.00	0.00	3A4
ATOM	3526	С	GLU	485	24.043	1.288	2.206	1.00	0.00	3A4
ATOM	3527	0	GLU	485	25.260	1.289	2.296	1.00	0.00	3A4 3A4
ATOM	3528	N	LYS	486	23.368	0.126	2.027 1.973	1.00	0.00	3A4
MOTA	3529	CA	LYS	486 486	24.038 23.286	-1.172 -2.272	2.791	1.00	0.00	3A4
ATOM ATOM	3530 3531	CB CG	LYS LYS	486	24.070	-3.558	3.141	1.00	0.00	. 3A4
MOTA	3532	CD	LYS	486	24.136	-4.672	2.074	1.00	0.00	3A4
ATOM	3533	CE	LYS	486	22.782	-5.249	1.626	1.00	0.00	3A4
ATOM	3534	NZ	LYS	486	22.037	-5.839	2.765	1.00	0.00	3A4.
MOTA	3535	C .	LYS	486	24.427	-1.507	0.545	1.00	0.00	3A4 3A4
ATOM	3536	0	LYS	486	25.595	-1.841 -1.396	0.334 -0.475	1.00	0.00	. 3A4
MOTA	3537 3538	N CA	PRO	487 487	23.564 23.980	-1.646	-1.846	1.00	0.00	3A4
MOTA MOTA	3539	CD	PRO	487	22.127	-1.666		1.00	0.00	3A4
MOTA	3540	СВ	PRO	487	22.967	-2.687	-2.354	1.00	0.00	3A4
ATOM	3541	CG	PRO	487	21.658	-2.329	-1.638	1.00	0.00	3A4
MOTA	3542	С	PRO	487	23.927	-0.353	-2.647	1.00	0.00	3A4 3A4
MOTA	3543	0	PRO	487	22.999	0.443	-2.510 -3.541	1.00	0.00	3A4
ATOM	3544	N	VAL	488	24.915 24.946	-0.147 1.001	-4.417	1.00	0.00	3A4
ATOM	3545 3546	CA CB	VAL VAL	488 488	25.614	2.234	-3.794	1.00	0.00	3A4
MOTA MOTA	3547		VAL	488	26.927	1.920	-3.030	1.00	0.00	3A4
ATOM	3548		VAL	488	25.731	3.431	-4.776	1.00	0.00	3A4
ATOM	3549	C	VAL	488	25.663	0.556	-5.657	1.00	0.00	3A4
ATOM	3550	0	VAL	488	26.886	0.485	-5.692	1.00	0.00	3A4 3A4
ATOM	3551	N	VAL	489	24.905	0.264	-6.743 -8.007		0.00	3A4
ATOM	3552	CA	VAL VAL	489 489	25.452 24.587	-0.202 -1.266	-8.687		0.00	3A4
ATOM ATOM	3553 3554	CB CG1	VAL	489	25.369	-1.938	-9.848			3A4
ATOM	3555		VAL	489	24.212	-2.339	-7.638		0.00	3A4
ATOM	3556	c	VAL	489	25.702	0.999	-8.916			3A4
MOTA	3557	0	VAL	489	24.854	1.864	-9.093	1.00	0.00	3A4

ATOM	3558	N	LEU	490	26.915	1.064 -9.499	1.00	0.00	3A4
MOTA	3559	CA	LEU	490	27.387	2.104 -10.386	1.00	0.00	3A4 3A4
ATOM	3560	CB	LEU	490 490	28.695 29.556	2.765 -9.828 3.732 -10.717	1.00	0.00 0.00	3A4
ATOM ATOM	3561 3562	CG CD1	LEU	490	30.364	4.675 -9.816	1.00	0.00	3A4
ATOM	3563	CD2		490	30.579	3.092 -11.694	1.00	0.00	3A4
MOTA	3564	С	LEU	490	27.689	1.443 -11.710	1.00	0.00	3A4
ATOM	3565	0	LEU	490	28.311 27.223	0.382 -11.714 2.080 -12.824	1.00	0.00	3A4 3A4
ATOM ATOM	3566 3567	N CA	LYS LYS	491 491	27.223	1.589 -14.188	1.00	0.00	3A4
ATOM	3568	CB	LYS	491	25.982	2.230 -14.965	1.00	0.00	3A4
ATOM	3569	CG	LYS	491	25.687	1.704 -16.388	1.00	0.00	3A4
ATOM	3570	CD	LYS	491	25.319	0.219 -16.460	1.00	0.00 0.00	3A4 3A4
ATOM	3571 3572	CE N2	LYS	491 491	25.043 24.678	-0.263 -17.889 -1.699 -17.899	1.00	0.00	3A4
ATOM ATOM	3573	C	LYS	491	28.494	1.812 -14.912	1.00	0.00	3A4
ATOM	3574	ō	LYS	491	29.380	0.964 -14.854	1.00	0.00	3A4
ATOM	3575	N	VAL	492	28.641	2.966 -15.620	1.00	0.00	3A4 3A4
ATOM	3576	CA	VAL	492 492	29.700 29.112	3.255 -16.574 3.889 -17.838	1.00	0.00	3A4
ATOM ATOM	3577 3578	CB CG1	VAL VAL	492	28.415	5.242 -17.560	1.00	0.00	3A4
ATOM	3579		VAL	492	30.130	3.946 -19.001	1.00	0.00	3A4
ATOM	3580	С	VAL	492	30.777	4.082 -15.898	1.00	0.00	3A4
ATOM	3581	0	VAL	492	30.519	4.769 -14.911 3.983 -16.415	1.00	0.00	3A4 3A4
ATOM ATOM	3582 3583	N CA	GLU	493 493	32.030 33.215	4.574 ~15.836	1.00	0.00	3A4
ATOM	3584	CB	GLU	493	33.962	3.566 -14.901	1.00	0.00	3A4
ATOM	3585	CG	GLU	493	34.397	2.206 -15.502	1.00	0.00	3A4
MOTA	3586	CD	GLU	493	35.792	2.272 -16.141	1.00	0.00	3A4 3A4
ATOM	3587 3588		GLU	493 493	36.769 35.901	2.568 -15.402 2.024 -17.372	1.00	0.00	3A4
ATOM ATOM	3589	C	GLU	493	34.100	5.031 -16.967	1.00	0.00	3A4
ATOM	3590	ō	GLU	493	33.928	4.629 -18.117	1.00	0.00	3A4
ATOM	3591	N	SER	494	35.109	5.874 -16.624	1.00	0.00	3A4 3A4
ATOM	3592	CA	SER	494 494	36.209 36.076	6.283 -17.480 7.748 -18.010	1.00	0.00 0.00	3A4
ATOM ATOM	3593 3594	CB OG	SER	494	35.765	8.692 -16.990	1.00	0.00	3A4
ATOM	3595	C	SER	494	37.455	6.059 -16.647	1.00	0.00	3A4
MOTA	3596	0	SER	494	37.360	5.784 -15.452	1.00	0.00	3A4 3A4
ATOM	3597	N	ARG	495 495	38.664 39.886	6.138 -17.262 5.740 -16.587	1.00	0.00	3A4
ATOM ATOM	3598 3599	CA CB	ARG	495	40.090	4.192 -16.590	1.00	0.00	3A4
ATOM	3600	CG	ARG	495	39.845	3.452 -17.916	1.00	0.00	3A4
ATOM	3601	CD	ARG	495	39.764	1.935 -17.697	1.00	0.00	3A4 3A4
ATOM	3602	NE	ARG	495	39.301 38.710	1.272 -18.966 0.032 -18.992	1.00	0.00	3A4
ATOM ATOM	3603 3604	CZ NH1	ARG ARG	495 495	38.289	-0.478 -20.185	1.00	0.00	3A4
ATOM	3605		ARG	495	38.527	-0.702 -17.853	1.00	0.00	3A4
MOTA	3606		ARG	495	41.073	6.436 -17.202	1.00	0.00	3A4 3A4
ATOM	3607	0	ARG	. 495 496	41.144 42.044	6.643 -18.413 6.804 -16.320	1.00	0.00	3A4
ATOM ATOM	3608 3609	N CA	ASP ASP	496	43.290	7.471 -16.647	1.00	0.00	3A4
MOTA	3610	СВ	ASP	496	43.159	9.025 -16.860	1.00	0.00	3A4
ATOM	3611	CG		496	42.410	9.788 -15.743	1.00	0.00	3A4 3A4
ATOM	3612		ASP	496 496	43.070 41.179	10.614 -15.056 9.574 -15.577	1.00	0.00	3A4
MOTA MOTA	3613 3614	C	ASP ASP	496	44.272	7.071 -15.553	1.00	0.00	3A4
ATOM	3615	ō	ASP	496	44.432	5.882 -15.283	1.00	0.00	3A4
ATOM	3616	N	GLY	497	44.958	8.050 -14.898	1.00	0.00	3A4 3A4
ATOM	3617	CA	GLY	497 497	45.950 46.123	7.790 -13.872 9.024 -13.031	1.00	0.00	3A4
ATOM ATOM	3618 3619	С 0	GLY GLY	497	46.262	10.127 -13.557	1.00	0.00	3A4
ATOM	3620	N	THR		46.127	8.846 -11.677	1.00	0.00	3A4
ATOM	3621	CA	THR		46.355	9.879 -10.674	1.00	0.00	3A4 3A4
ATOM	3622	CB	THR		45.075 44.194	10.401 -9.995 9.349 -9.600	1.00	0.00	3A4 3A4
ATOM ATOM	3623 3624		THR		44.332	11.355 -10.957		0.00	3A4
ATOM	3625	c	THR		47.290	9.274 -9.640	1.00	0.00	3A4
ATOM	3626	0	THR		47.189	8.089 -9.326		0.00	3A4 3A4
ATOM	3627	N	VAL		48.205 49.121	10.109 -9.074 9.727 -8.014			3A4 3A4
ATOM ATOM	3628 3629	CA CB	VAL		50.272	8.816 -8.476			3A4

ATOM	3630	CG1	VAL	499 .	51.133	9.436	-9.607	1.00	0.00		3A4
ATOM	3631		VAL	499	51.110	8.313	-7.273	1.00	0.00		3A4
				499	49.614	11.021	-7.391	1.00	0.00		3A4
MOTA	3632	C	VAL								3A4
MOTA	3633	0	VAL	499	49.977	11.961	-8.097	1.00	0.00		
ATOM	3634	N	SER	500	49.647	11.075	-6.030	1.00	0.00		3A4
ATOM	3635	CA	SER	500	50.251	12.152	-5.269	1.00	0.00		3A4
MOTA	3636	СВ	SER	500	49.434	13.486	-5.230	1.00	0.00		3A4
ATOM	3637	OG	SER	500	48.086	13.306	-4.816	1.00	0.00		3A4
		C		500	50.524	11.618	-3.882	1.00	0.00		3A4
ATOM	3638		SER					1.00	0.00		3A4
ATOM	3639	0	SER	500	49.694	10.933	-3.286				
ATOM	3640	N	GLY	501	51.736	11.945	-3.355	1.00	0.00		3A4
ATOM	3641	CA	GLY	501	52.249	11.543	-2.061	1.00	0.00		3A4
ATOM	3642	C	GLY	501	53.489	10.727	-2.291	1.00	0.00		3A4
ATOM	3643	0	GLY	501	54.576	11.087	-1.841	1.00	0.00		3A4
ATOM	3644	N	ALA	502	53.331	9.596	-3.020	1.00	0.00		3A4
					54.406	8.722	-3.424	1.00	0.00		3A4
MOTA	3645	CA	ALA	502			-				
ATOM	3646	СВ	ALA	502	54.772	7.642	-2.379	1.00	0.00		3A4
MOTA	3647	С	ALA	502	53.912	8.031	-4.704	1.00	0.00		3A4
MOTA	3648	OT1	ALA	502	54.439	8.364	-5.800	1.00	0.00		3A4
MOTA	3649	OT2	ALA	502	52.987	7.178	-4.607	1.00	0.00		3A4
TER	3650		ALA	502							
HETATM		FE	HEM	600	33.118	10.391	15.288	1.00	0.00		HEM
									0.00		HEM
HETATM		NA	HEM	600	31.497	11.115	16.171	1.00			
HETATM		NB	HEM	600	32.274	10.658	13.514	1.00	0.00		HEM
HETATM	3654	NC	HEM	600	34.752	9.684	14.430	1.00	0.00		HEM
HETATM	3655	ND	HEM	600	33.949	10.106	17.065	1.00	0.00		HEM
HETATM			HEM	600	31.254	11.251	17.515	1.00	0.00		HEM
НЕТЛТМ			HEM	600	29.887	11.659	17.752	1.00	0.00		HEM
HETATM				600	29.316	11.871	16.542	1.00	0.00		HEM
			HEM								
НЕТАТМ			HEM	600	30.322	11.523	15.568	1.00	0.00		HEM
HETATM			HEM	600	31.012	11.136	13.233	1.00	0.00		HEM
HETATM	3661	C2B	HEM	600	30.761	11.218	11.804	1.00	0.00		HEM
HETATM	3662	СЗВ	HEM	600	31.901	10.761	11.185	1.00	0.00		HEM
HETATM	3663		HEM	600	32.828	10.426	12.273	1.00	0.00		HEM
HETATM			HEM	600	35.044	9.645	13.089	1.00	0.00		HEM
				600	36.395	9.168	12.838	1.00	0.00		HEM
HETATM			HEM								
HETATM			HEM	600	36.920	8.833	14.067	1.00	0.00		HEM
HETATM			HEM	600	35.879	9.167	15.033	1.00	0.00		HEM
HETATM	3668	ClD	HEM	600	35.150	9.494	17.358	1.00	0.00		HEM
HETATM	3669	C2D	HEM	600	35.382	9.408	18.787	1.00	0.00		HEM
HETATM	3670	C3D	HEM	600	34.329	10.035	19.375	1.00	0.00	·	HEM
HETATM			HEM	600	33.438	10.439	18.306	1.00	0.00		HEM
HETATM			HEM	600	32.186	10.978	18.500	1.00	0.00		HEM
									0.00	•	
HETATM			HEM	600	30.115	11.530	14.204	1.00			HEM
HETATM			HEM	600	34.131	9.963	12.102	1.00	0.00		HEM
HETATM	3675	CHD	HEM	600	36.032	9.062	16.407	1.00	0.00		HEM
HETATM	3676	CMA	HEM	600	27.911	12.344	16.281	1.00	0.00		HEM
HETATM	3677	CAA	HEM	600	29.208	11.695	19.088	1.00	0.00		HEM
HETATM	3678		HEM	600	29,154	13.045	19.638	1.00	0.00	•	HEM
HETATM			HEM	600	28.459	13.237	20.946		0.00		HEM
HETATM		-	HEM	600	28.097	12.278	21.566	1.00	0.00		HEM
HETATM			HEM	600	28.217	14.323	21.438		0.00		HEM
HETATM	3682	CMB	HEM	600	29.483	11.742	11.185	1.00	0.00		HEM
HETATM	3683	CAB	HEM	600	32.219	10.602	9.818	1.00	0.00		HEM
HETATM	3684		HEM	600	31.527	10.978	8.735	1.00	0.00		HEM
HETATM			HEM	600	37.047	9.116	11.471	1.00	0.00	•	HEM
HETATM			HEM	600	38.159	8.288	14.465	1.00	0.00		HEM
HETATM			HEM	600	39.265	8.069	13.758	1.00	0.00		HEM
HETATM			HEM	600	36.499	8.680	19.483	1.00	0.00		HEM
HETATM	3689	CAD	HEM	600	34.101	10.253	20.849	1.00	0.00		HEM
HETATM	3690	CBD	HEM	600	34.689	11.583	21.366	1.00	0.00		HEM
HETATM			HEM	600	34.355	11.863	22.843	1.00	0.00		HEM
HETATM			HEM	600	35.050	12.735	23.424	1.00	0.00		HEM
HETATM			HEM	600	33.381	11.284	23.380	1.00	0.00		HEM
	2023	<b>U2</b> D	11017	300	JJ. JOI	11.204	23.300	1.00			
END											

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Table 4: Providing the coordinates of the CYP3A model
          CYP3A7
HEADER
          MODEL OF HUMAN CYTOCHROME P450 CYP3A7
TITLE
          N. LOISEAU, F. ANDRE, M. DELAFORGE, M. COTTEVIEILLE
AUTHOR
                    PRO PHE LEU GLY ASN ALA LEU SER PHE ARG LYS GLY TYR
SEQRES
         1
               459
                    TRP THR PHE ASP MET GLU CYS TYR LYS LYS TYR ARG LYS
SEORES
               459
SEQRES
               459
                    VAL TRP GLY ILE TYR ASP CYS GLN GLN PRO MET LEU ALA
                    ILE THR ASP PRO ASP MET ILE LYS THR VAL LEU VAL LYS
SEQRES
         4
               459
                    GLU CYS TYR SER VAL PHE THR ASN ARG ARG PRO PHE GLY
SEORES
         5
               459
                    PRO VAL GLY PHE MET LYS ASN ALA ILE SER ILE ALA GLU
SEQRES
         6
               459
                    ASP GLU GLU TRP LYS ARG ILE ARG SER LEU LEU SER PRO
SEORES
         7
               459
                    THR PHE THR SER GLY LYS LEU LYS GLU MET VAL PRO ILE
SEQRES
         8
               459
                    ILE ALA GLN TYR GLY ASP VAL LEU VAL ARG ASN LEU ARG
SEQRES
         9
               459
                    ARG GLU ALA GLU THR GLY LYS PRO VAL THR LEU LYS HIS
SEQRES
         10
               459
                    VAL PHE GLY ALA TYR SER MET ASP VAL ILE THR SER THR
SEORES
        11
               459
                    SER PHE GLY VAL SER ILE ASP SER LEU ASN ASN PRO GLN
SEQRES
        12
               459
SEQRES
        13
               459
                    ASP PRO PHE VAL GLU ASN THR LYS LYS LEU LEU ARG PHE
                    ASN PRO LEU ASP PRO PHE VAL LEU SER ILE LYS VAL PHE
SEORES
        14
               459
                    PRO PHE LEU THR PRO ILE LEU GLU ALA LEU ASN ILE THR
SEORES
        15
               459
                    VAL PHE PRO ARG LYS VAL ILE SER PHE LEU THR LYS SER
SEQRES
        16
               459
                    VAL LYS GLN ILE LYS GLU GLY ARG LEU LYS GLU THR GLN
SEQRES
        17
               459
                    LYS HIS ARG VAL ASP PHE LEU GLN LEU MET ILE ASP SER
SEQRES
               459
        18
SEQRES
                    GLN ASN SER LYS ASP SER GLU THR HIS LYS ALA LEU SER
        19
               459
                    ASP LEU GLU LEU MET ALA GLN SER ILE ILE PHE ILE PHE
SEQRES
        20
               459
                    ALA GLY TYR GLU THR THR SER SER VAL LEU SER PHE ILE
SEQRES
        21
               459
                    ILE TYR GLU LEU ALA THR HIS PRO ASP VAL GLN GLN LYS
SEORES
        22
               459
SECRES
        23
               459
                    VAL GLN LYS GLU ILE ASP THR VAL LEU PRO ASN LYS ALA
                    PRO PRO THR TYR ASP THR VAL LEU GLN LEU GLU TYR LEU
SEORES
        24
               459
                    ASP MET VAL VAL ASN GLU THR LEU ARG LEU PHE PRO VAL
SEQRES
        25
               459
                    ALA MET ARG LEU GLU ARG VAL CYS LYS LYS ASP VAL GLU
SEQRES
        26
               459
                    ILE ASN GLY MET PHE ILE PRO LYS GLY VAL VAL WAT
SEQRES
        27
               459
                    ILE PRO SER TYR VAL LEU HIS HIS ASP PRO LYS TYR TRP
SEQRES
        28
               459
SEQRES
                    THR GLU PRO GLU LYS PHE LEU PRO GLU ARG PHE SER LYS
               459
SEQRES
                    LYS ASN LYS ASP ASN ILE ASP PRO TYR ILE TYR THR PRO
        30
               459
                    PHE GLY SER GLY PRO ARG ASN CYS ILE GLY MET ARG PHE
SEQRES
        31
                    ALA LEU VAL ASN MET LYS LEU ALA LEU VAL ARG VAL LEU
SEQRES
        32
               459
                    GLN ASN PHE SER PHE LYS PRO CYS LYS GLU THR GLN ILE
               459
SEQRES
        33
                    PRO LEU LYS LEU ARG PHE GLY GLY LEU LEU THR GLU
SEORES
        34
               459
                    LYS PRO ILE VAL LEU LYS ALA GLU SER ARG ASP GLU THR
SEORES
        35
               459
                    VAL SER GLY ALA
SEORES
        36
               459
HET
       HEM
               600
HETNAM HEM
               HEME
               3,7,12,17-TETRAMETHYL-8,13-DIVINYL-2,18-PORPHINEDIPROPIONIC ACID
HETSYN HEM
FORMUL HEM
               C34 H34 N4 O4 FE1
                  PRO
                         45
                                  24.768
                                           6.244 -5.895 1.00
                                                                 0.00
                                                                               3A7
ATOM
              N
                                                  -4.648 1.00
MOTA
             CD
                  PRO
                         45
                                  25.053
                                           5.448
                                                                 0.00
                                                                               3A7
                                           5.319
                                                  -7.064
                                                                 0.00
                                                                               3A7
MOTA
          3
                         45
                                 24.705
                                                           1.00
             CA
                  PRO
                                                                 0.00
                                                                               3A7
             CB
                  PRO
                         45
                                 24.467
                                           3.950
                                                  -6.422
                                                           1.00
ATOM
                                           4.018
                                                  -5.139
                                                           1.00
                                                                 0.00
                                                                               3A7
ATOM
          5
             CG
                  PRO -
                         45 .
                                 25.292
                                 23.594
                                           5.801
                                                  -7.950
                                                           1.00
                                                                 0.00
                                                                               3A7
ATOM
          6
             С
                  PRO
                         45
                                                  -8.057
                                                                 0.00
                                                                               3A7
                                           7.010
                                                           1.00
ATOM
          7
             0
                  PRO
                         45
                                 23.387
                                                                               3A7
ATOM
          8
             N
                  PHE
                         46
                                 22.870
                                           4.857
                                                  -B.600
                                                           1.00
                                                                 0.00
                                                                 0.00
                                                                               3A7
MOTA
          9
             CA
                         46
                                 21.751
                                           5.140
                                                 -9.472
                                                           1.00
                  PHE
                                                                               3A7
ATOM
         10
             CB
                  PHE
                         46
                                 21.853
                                           4.416 -10.835
                                                           1.00
                                                                 0.00
MOTA
         11
             CG
                  PHE
                         46
                                  23.083
                                           4.887 -11.553
                                                           1.00
                                                                 0.00
                                                                               3A7
                                           4.033 -11.730
                                                           1.00
                                                                 0.00
                                                                               3A7
ATOM
         12
             CD1 PHE
                         46
                                  24.173
                                           6.189 -12.049
                                                           1.00
                                                                 0.00
                                                                               3A7
             CD2 PHE
                                  23.155
ATOM
         13
                         46
                                           4.474 -12.390
                                                                 0.00
                                                                               3A7
                                  25.317
                                                           1.00
ATOM
         14
             CE1
                  PHE
                         46
                                                                               3A7
                                  24.297
                                           6.633 -12.709
                                                           1.00
                                                                 0.00
         15
ATOM
             CE2
                  PHE
                         46
                                                                               3A7
                                           5.775 -12.879
                                                           1.00
                                                                 0.00
ATOM
         16
             CZ
                  PHE
                         46
                                  25.380
                                           4.691 -8.782
                                                                 0.00
                                                                               3A7
                                 20,491
                                                           1.00
ATOM
         17
             С
                  PHE
                         46
                                  19.400
                                           5.166
                                                  -9.096
                                                           1.00
                                                                 0.00
                                                                               3A7
ATOM
         18
             0
                  PHE
                         46
                                                 -7.814
                                                                               3A7
                                                           1.00
                                                                 0.00
MOTA
         19
             N
                  LEU
                         47
                                 20.629
                                           3.749
                                                                 0.00
                                                                               3A7
MOTA
         20
                         47
                                  19.541
                                           3.204
                                                  -7.035
                                                           1.00
             CA
                  LEU
                                                                               3A7
         21
                                  19.661
                                           1.667
                                                  -6.874
                                                           1.00
                                                                 0.00
ATOM
             CB
                  LEU
                         47
MOTA
         22
             CG
                  LEU
                                  18.490
                                           0.978
                                                   -6.129
                                                           1.00
                                                                 0.00
                                                                               3A7
ATOM
         23
             CD1 LEU
                         47
                                  17.133
                                           1.202
                                                  -6.826
                                                           1.00
                                                                 0.00
                                                                               7A7
                                          -0.526
                                                   -5.942
                                                           1.00
                                                                 0.00
                                                                               3A7
                                  18.768
MOTA
         24
             CD2 LEU
                         47
                                                                               3A7
                                  19.573
                                           3.860
                                                   -5.681
                                                           1.00
                                                                 0.00
         25
                  LEU
                         47
ATOM
             С
                                                  -5.036
                                                           1.00
                                                                 0.00
                                                                               3A7
                                  20.619
ATOM
         26
             0
                  LEU
                         47
                                           3.930
                                                                 0.00
                                                                               3A7
                                                   -5.225
                                                           1.00
ATOM
         27
              N
                  GLY
                         48
                                  18.396
                                           4.349
                                                                 0.00
                                                                               3A7
ATOM
         28
             CA
                  GLY
                         48
                                  18.240
                                           4.966
                                                  -3.933
                                                           1.00
```

ATOM	29	С	GLY	48	16.930	4.491	-3.395	1.00	0.00	3A7
ATOM	30	0	GLY	48	15.938	5.218	-3.414	1.00	0.00	3A7 3A7
MOTA	31 32	N CA	ASN ASN	49 49	16.911 15.741	3.229 2.585	-2.898 -2.348	1.00	0.00	3A7
ATOM ATOM	33	CB	ASN	49	15.445	1.235	-3.059	1.00	0.00	3A7
ATOM	34	CG	ASN	49	14.046	0.705	-2.706	1.00	0.00	3A7
ATOM	35	OD1	ASN	49	13.035	1.349	-3.011	1.00	0.00	3A7
ATOM	36		ASN	49	14.005	-0.494	-2.051	1.00	0.00	3A7 3A7
ATOM	37	C	ASN	49	16.016 17.169	2.375 2.278	-0.880 -0.463	1.00	0.00	3A7
ATOM ATOM	38 39	N	ASN ALA	49 50	14.933	2.293	-0.065	1.00	0.00	3A7
ATOM	40	CA	ALλ	50	14.998	2.111	1.369	1.00	0.00	3A7
ATOM	41	СВ	ALA	50	13.847	2.834	2.098	1.00	0.00	3A7
MOTA	42	С	ALA	50	14.941	0.641	1.697	1.00	0.00	3A7 3A7
ATOM	43	0	ALA	50	13.866 16.133	0.049 0.032	1.787 1.885	1.00	0.00	3A7
ATOM ATOM	44 45	N CA	LEU	51 51	16.271	-1.360	2.232	1.00	0.00	3A7
ATOM	46	CB	LEU	51	16.271	-2.314	1.001	1.00	0.00	3A7
ATOM	47	CG	LEU	51	17.055	-1.862	~0.262	1.00	0.00	3A7
MOTA	48		LEU	51	18.587	-1.811	-0.098	1.00	0.00	3A7 3A7
ATOM	49		LEU	· 51	16.690	-2.765 -1.468	-1.456 3.012	1.00	0.00	3A7 3A7
MOTA MOTA	50 51	C O	LEU	51 51	17.550 18.327	-0.517	3.085	1.00	0.00	3A7
ATOM	52	N	SER	52	17.794	-2.657	3.613	1.00	0.00	3A7
ATOM	53	CA	SER	52	19.005	-2.956	4.343	1.00	0.00	3A7
MOTA	54	CB	SER	52	18.741	-3.361	5.821	1.00	0.00	3A7
ATOM	55	OG	SER	52	17.737	-4.363	5.945 3.562	1.00	0.00	3A7 3A7
ATOM ATOM	56 57	С 0	SER	52 52	19.734 20.164	-4.023 -3.782	2.435	1.00	0.00	3A7
ATOM	58	N	PHE	53	19.898	-5.231	4.155	1.00	0.00	3A7
ATOM	59	CA	PHE	53	20.599	-6.341	3.550	1.00	0.00	3A7
ATOM	60	CB	PHE	53	21.908	-6.703	4.297	1.00	0.00	3A7
ATOM	61	CG	PHE	53	22.730	-5.456 -4.809	4.439 5.673	1.00	0.00	3A7 3A7
ATOM ATOM	62 63		PHE	53 53	22.819 23.346	~4.880	3.327	1.00	0.00	3A7
ATOM	. 64		PHE	53	23.491	3.598	5.793	1.00	0.00	3A7
ATOM	65		PHE	53	24.018	-3.667	3.446	1.00	0.00	3A7
ATOM	66	CZ	PHE	53	24.085	-3.022	4.675	1.00	0.00	3A7
ATOM	67	C	PHE	53	19.639	-7.494	3.594	1.00	0.00	3A7 3A7
ATOM ATOM	68 69	O N	PHE	53 54	19.885 18.491	-8.495 -7.330	4.264 2.875	1.00	0.00	3A7
ATOM	70	CA	ARG	54	17.327	-8.205	2.828	1.00	0.00	3A7
ATOM	71	СВ	ARG	54	17.629	-9.719	2.641	1.00	0.00	3A7
MOTA	72	CG	ARG	54	18.536		1.437	1.00	0.00	3A7
ATOM	73	CD.	ARG	54	17.996 19.049	-9.573 -9.836	0.079	1.00	0.00	3A7 3A7
MOTA MOTA	74 75	NE CZ	ARG ARG	54 54	19.036		-1.791	1.00	0.00	3A7
ATOM	76		ARG	54		-11.113	-2.669	1.00	0.00	3A7
MOTA	77		ARG	54	18.013	-11.826	-1.753	1.00	0.00	3A7
ATOM	78	С	ARG	54	16.514	-7.983	4.087	1.00	0.00	3A7 3A7
ATOM	79	0	ARG	5 <i>4</i> 55	16.760 15.545	-8.611 -7.030	5.116 4.028	1.00	0.00	3A7
MOTA MOTA	80 81	N CA	LYS LYS	55 55	14.927	-6.447	5.205	1.00	0.00	3A7
ATOM	82	СВ	LYS	55	14.520	-4.971	5.023	1.00	0.00	3A7
MOTA	83	CG	LYS	55	13.327	-4.656	4.092	1.00	0.00	3A7
ATOM	84	CD	LYS	55	13.574	-4.842	2.582	1.00	0.00	3A7 3A7
MOTA MOTA	85 86	CE NZ	LYS LYS	55 55	13.074 11.612	-6.171 -6.322	1.993 2.178	1.00	0.00	3A7
ATOM	87	C	LYS	55	13.767	-7.241	5.777	1.00	0.00	3A7
ATOM	88	ō	LYS	55	13.403	-7.067	6.938	1.00	0.00	3A7
ATOM	89	N	GLY	56	13.158	-8.146	4.991	1.00	0.00	3A7
ATOM	90	CA	GLY	56	12.066		5.491	1.00	0.00	3A7 3A7
ATOM	91 92	C O	GLY GLY	56 56		-10.146 -10.334	4.604 3.823	1.00	0.00	3A7
ATOM ATOM	93	N	TYR	56 57		-11.031	4.730	1.00	0.00	3A7
ATOM	94	CA	TYR	57	13.171	-12.222	3.922	1.00	0.00	3A7
ATOM	95	CB	TYR	57		-12.913	4.319	1.00	0.00	3A7
ATOM	96	CG	TYR	57		-13.558	3.146	1.00	0.00	3A7 3A7
MOTA	97 98		TYR TYR	57 57		-12.832 -14.898	1.995 3.223	1.00	0.00	3A7
MOTA MOTA	98		TYR	57		-13.440	0.934	1.00	0.00	3A7
ATOM	100		TYR	57		-15.506	2.168	1.00	0.00	3A7

ATOM	101	CZ	TYR	57	16.538	-14.777	1.021	1.00	0.00	3A7
ATOM	102	OH	TYR	57		-15.392	-0.043	1.00	0.00	3A7
ATOM	103	С	TYR	57	12.013	-13.191	4.022	1.00	0.00	3A7
ATOM	104	0	TYR	57		-13.781	3.021	1.00	0.00	3A7
ATOM	105	N	TRP	58		-13.353	5.211	1.00	0.00	3A7
ATOM	106	CA	TRP	58		-14.269	5.359	1.00	0.00	3A7
MOTA	107	СВ	TRP	58		-14.515	6.832	1.00	0.00	3A7 3A7
ATOM	108	CG	TRP	58		-13.318	7.606	1.00	0.00	3A7
ATOM	109		TRP	58		-13.247	8.157 7.871	1.00	0.00	3A7
ATOM	110 111		TRP	58 58		-12.115 -11.297	8.548	1.00	0.00	3A7
ATOM ATOM	112		TRP	58		-11.978	8.741	1.00	0.00	3A7
ATOM	113			58		-14.158	8.175	1.00	0.00	3A7
ATOM	114		TRP	58		-11.604	9.360	1.00	0.00	3A7
ATOM	115		TRP	58		-13.780	8.796	1.00	0.00	3A7
ATOM	116	CH2	TRP	58	5.647	-12.522	9.382	1.00	0.00	3A7
ATOM	117	С	TRP	58	9.036	-13.824	4.612	1.00	0.00	3A7
ATOM	118	0	TRP	58		-14.664	4.106	1.00	0.00	3A7
MOTA	119	N	THR	59		-12.490	4.502	1.00	0.00	3A7
ATOM	120	CA	THR	59		-11.989	3.737	1.00	0.00	3A7 3A7
ATOM	121	CB	THR	59		-10.582	4.136	1.00	0.00	3A7 3A7
ATOM	122		THR	59 50	8.282	-9.643	4.073 5.579	1.00	0.00	3A7
ATOM	123		THR	59 59		-10.634 -12.067	2.267	1.00	0.00	3A7
ATOM ATOM	124 125	С 0	THR	59		-12.232	1.471	1.00	0.00	3A7
ATOM	126	N	PHE	60		-12.018	1.884	1.00	0.00	3A7
ATOM	127	CA	PHE	60		-12.244	0.530	1.00	0.00	3A7
ATOM	128	СВ	PHE	60	-	-11.803	0.330	1.00	0.00	3A7
ATOM	129	CG	PHE	60		-11.735	-1.126	1.00	0.00	3A7
ATOM	130	CD1	PHE	60	10.889	-10.822	-1.978	1.00	0.00	3A7
ATOM	131	CD2	PHE	60		-12.595	-1.647	1.00	0.00	3A7
ATOM	132		PHE	60		-10.772	-3.328	1.00	0.00	3A7
ATOM	133		PHE	60		-12.548	-2.997	1.00	0.00	3A7
MOTA	134	CZ	PHE	60		-11.636	-3.839	1.00	0.00	3A7
ATOM	135	С	PHE	60		-13.695	0.122	1.00	0.00	3A7 3A7
MOTA	136	0	PHE	60 61		-14.011 -14.632	-0.936 0.991	1.00	0.00	3A7
ATOM ATOM	137 138	N CA	ASP ASP	61 61		-14.052	0.737	1.00	0.00	3A7
ATOM	139	CB	ASP	61		-16.892	1.774	1.00	0.00	3A7
ATOM	140	CG	ASP	61		-16.729	1.612	1.00	0.00	3A7
ATOM	141		ASP	61		-16.736	0.447	1.00	0.00	3A7
ATOM	142		ASP	61		-16.555	2.655	1.00	0.00	3A7
ATOM	143	С	ASP	61	8.415	-16.503	0.698	1.00	0.00	- 3A7
ATOM	. 144	0	ASP	61		-17.371	-0.085	1.00	0.00	3A7
ATOM	145	N	MET	62		-15.870	1.491	1.00	0.00	3A7
ATOM	146	CA	MET	62		-16.134	1.452	1.00	0.00	3A7 3A7
ATOM	147	CB	MET	62		-15.468		1.00	0.00	3A7
ATOM	148	CG SD	MET	62 62		-16.224 -15.359	3.947 5.422	1.00	0.00	3A7
ATOM ATOM	149 150	CE	MET MET	62		-15.481	5.031	1.00	0.00	3A7
ATOM	151	C	MET	62		-15.672	0.168	1.00	0.00	3A7
ATOM	152	ŏ	MET	62		-16.335	-0.342	1.00	0.00	3A7
ATOM	153	N	GLU	63	5.922	-14.555	-0.430	1.00	0.00	3A7
ATOM	154	CA	GLU	63	5.457	-14.094	-1.722	1.00	0.00	3A7
MOTA	155	CB	GLU	63		-12.683	-2.039	1.00	0.00	3A7
MOTA	156	CG	GLU	63		-11.593	-1.206	1.00	0.00	3A7
MOTA	157	CD	GLU	63		-10.239	-1.427	1.00	0.00	3A7
MOTA	158		GLU	63		-10.169	-2.214	1.00	0.00	3A7 3A7
ATOM	159		GLU	63	5.495	-9.249	-0.802	1.00	0.00	3A7
ATOM	160	C	GLU	63		-15.044	-2.831	1.00	0.00	3A7
ATOM ATOM	161 162	и О	GLU CYS	63 64		-15.339 -15.606	-3.734 -2.747	1.00	0.00	3A7
ATOM	163	CA	CYS	64		-16.598	-3.674	1.00	0.00	3A7
ATOM	164	CB	CYS	64		-16.969	-3.362	1.00	0.00	3A7
MOTA	165	SG	CYS	64		-15.524	-3.736	1.00	0.00	3A7
ATOM	166	c	CYS	64		-17.853	-3.631	1.00	0.00	3A7
ATOM	167	ō	CYS	64	6.413	-18.402	-4.655	1.00	0.00	3A7
ATOM	168	N	TYR	65		-18.323	-2.413	1.00	0.00	3A7
ATOM	169	CA	TYR	65		-19.526	-2.251	1.00	0.00	3A7
ATOM	170	ÇВ	TYR	65		-19.993	-0.802	1.00	0.00	3A7
ATOM	171	CG	TYR	65		-20.246	-0.379	1.00	0.00	3A7
ATOM	172	CD1	TYR	65	7.458	-19.725	0.834	1.00	0.00	3A7

ATOM	173	CD2	TYR	65	7.985	-20.850	-1.222	1.00	0.00	3A7
ATOM	174	CE1	TYR	65	8.800	-19.750	1.182	1.00	0.00	3A7
ATOM	175	CE2	TYR	65		-20.816	-0.901	1.00	0.00	3A7
ATOM	176	CZ	TYR	65		-20.216	0.283	1.00	0.00	3A7
ATOM	177	ОН	TYR	65		-20.003	0.572	1.00	0.00	3A7
MOTA	178	C	TYR	65		-19.373	-2.701	1.00	0.00	3A7
ATOM	179	0	TYR	65		-20.319	-3.228	1.00	0.00	3A7 3A7
ATOM	180	N	LYS	66 66		-18.174 -17.922	-2.556 -3.043	1.00	0.00	3A7
ATOM	181 182	CA CB	LYS LYS	66 66		-16.564	-2.544	1.00	0.00	3A7
ATOM ATOM	183	CG	LYS	66		-16.579	-1.049	1.00	0.00	3A7
ATOM	184	CD	LYS	66		-15.185	-0.470	1.00	0.00	3A7
ATOM	185	CE	LYS	66		-14.502	-1.089	1.00	0.00	3 <b>A</b> 7
ATOM	186	NZ	LYS	66		-13.182	-0.461	1.00	0.00	3 <b>a</b> 7
ATOM	187	С	LYS	66	2.244	-17.957	-4.556	1.00	0.00	3A7
ATOM	188	0	LYS	66	1.227	-18.326	-5.129	1.00	0.00	3A7
ATOM	189	N	LYS	67	3.349	-17.595	-5.243	1.00	0.00	3A7
MOTA	190	CA	LYS	67		-17.539	-6.682	1.00	0.00	3A7
ATOM	191	CB	LYS	67		-16.414	-7.137	1.00	0.00	3A7
ATOM	192	CG	LYS	67		-16.145	-8.651	1.00	0.00	3A7
ATOM	193	CD	LYS	67		-14.878	-9.034	1.00	0.00	3A7 3A7
ATOM	194	CE	LYS	67 67		-14.629 -14.424		1.00	0.00	3A7 3A7
ATOM ATOM	195 196	NZ C	LYS LYS	67		-18.855	-7.284	1.00	0.00	3A7
ATOM	197	Ö	LYS	67		-19.336	-8.244	1.00	0.00	3A7
ATOM	198	N	TYR	68		~19.451	-6.748	1.00	0.00	3A7
ATOM	199	CA	TYR	68		-20.573	-7.355	1.00	0.00	3A7
ATOM	200	СВ	TYR	68		-20.402	-7.314	1.00	0.00	3A7
ATOM	201	CG	TYR	68	7.522	-19.259	-8.216	1.00	0.00	3A7
ATOM	202	CD1	TYR	68	7.789	-17.989	-7.702	1.00	0.00	3A7
ATOM	203	CD2	TYR	68		-19.457	-9.595	1.00	0.00	3A7
ATOM	204		TYR	68		-16.937	-8.550	1.00	0.00	3A7
ATOM	205		TYR	68		-18.408		1.00	0.00	3A7
ATOM	206	CZ	TYR	68		-17.146	-9.924	1.00	0.00	3A7
ATOM	207	OH	TYR	68		-16.080 -21.899	-6.770	1.00	0.00	3A7 · 3A7
ATOM ATOM	208 209	С О	TYR TYR	68 68		-22.918	-7.453	1.00	0.00	3A7
ATOM	210	N	ARG	69		-21.912	-5.500	1.00	0.00	3A7
ATOM	211	CA	ARG	69		-23.040	-4.856	1.00	0.00	3A7
ATOM	212	СВ	ARG	69		-23.733	-5.717	1.00	0.00	3A7
ATOM	213	CG	ARG	69		-22.762	-6.180	1.00	0.00	3A7
ATOM	214	CD	ARG	69	0.844	-23.441	-7.009	1.00	0.00	3A7
ATOM	215	NE	ARG	69		-23.933	-8.287	1.00	0.00	3A7
MOTA	216	CZ	ARG	69		-24.664	-9.197	1.00	0.00	3A7
ATOM	217	NH1		69		-25.083		1.00	0.00	3A7
ATOM	218	NH2		69		-24.981	-8.963	1.00	0.00	3A7
MOTA	219	C	ARG	69		-23.968	-4.257	1.00	0.00	3A7 3A7
ATOM ATOM	220 221	О . И	ARG	- 69 - 70		-23.556 -25.251	-3.663 -4.585	1.00	0.00	3A7
ATOM .	222	CA.	LYS LYS	70		-26.459	-4.410	1.00	0.00	3A7
ATOM	223	СВ	LYS	70		-27.726	-4.955	1.00	0.00	3A7
ATOM	224	CG	LYS	70		-28.142		1.00	0.00	3A7
ATOM	225	CD	LYS	70		-27.345	-4.536	1.00	0.00	3A7
MOTA	226	CE	LYS	70	1.635	-27.577	-5.929	1.00	0.00	3A7
MOTA	227	NZ	LYS	70		-26.976	-7.009	1.00	0.00	3A7
ATOM	228	С	LYS	70		-26.352	-5.122	1.00	0.00	3A7
MOTA	229	0	LYS	70		-26.860	-6.233	1.00	0.00	3A7
MOTA	230	N	VAL	71		-25.662	-4.449	1.00	0.00	3A7
MOTA	231	CA	VAL	71		-25.641	-4.770	1.00	0.00	3A7
ATOM	232	CB	VAL	71		-26.967	-5.362	1.00	0.00	3A7
ATOM	233 234	CG1		71 71		-26.882 -28.158	-5.635 -4.411	1.00	0.00	3A7 3A7
ATOM ATOM	234	CG2 C	VAL	71 71		-28.138	-5.708	1.00	0.00	3A7
ATOM	236	Ö	VAL	71		-24.376	-6.751	1.00	0.00	3A7
ATOM	237	N	TRP	72		-23.545	-5.337	1.00	0.00	3A7
ATOM	238	CA	TRP	72		-22.433	-6.182	1.00	0.00	3A7
ATOM	239	СВ	TRP	72		-21.089	-5.839	1.00	0.00	3A7
ATOM	240	CG	TRP	72		-19.873	-5.306	1.00	0.00	3A7
ATOM	241	CD2		72		-18.737	-6.108	1.00	0.00	3A7
MOTA	242	CD1		72		-19.633	-4.054	1.00	0.00	3A7
ATOM	243	NE1		72		-18.438	-4.024	1.00	0.00	3A7
MOTA	244	CE2	TRP	72	11.871	-17.866	-5.277	1.00	0.00	3A7

ATOM	245	CE3	TRP	72	10.923	-18.434	-7.436	1.00	0.00	3A7
ATOM	246		TRP	72	12.368	-16.672	-5.760	1.00	0.00	3A7
ATOM	247		TRP	72		-17.223	-7.920	1.00	0.00	3A7
ATOM	248		TRP	72		-16.354	-7.094	1.00	0.00	3A7
ATOM	249	C	TRP	72		-22.293	-6.064	1.00	0.00	3A7
				72		-22.782	-5.112	1.00	0.00	3A7
ATOM	250	0	TRP							3A7
ATOM	251	N	GLY	73		-21.582	-7.022	1.00	0.00	
MOTA	252	CA	GLY	73		-21.323	-6.985	1.00	0.00	3A7
ATOM	253	С	GLY	73		-19.850	-6.821	1.00	0.00	3A7
ATOM	254	0	GLY	73	13.812	-19.031	-7.409	1.00	0.00	3A7
ATOM	255	N	ILE	74	15.530	~19.484	-6.009	1.00	0.00	3A7
ATOM	256	CA	ILE	74	15.929	~18.120	-5.754	1.00	0.00	3A7
ATOM	257	CB	ILE	74	15.600	-17.676	-4.328	1.00	0.00	3A7
ATOM	258		ILE	74		-18.543	-3.258	1.00	0.00	3A7
ATOM	259		ILE	74		-16.159	-4.124	1.00	0.00	3A7
ATOM	260	CD	ILE	74		-15.621	-2.836	1.00	0.00	3A7
ATOM	261	c	ILE	74		-18.077	-6.023	1.00	0.00	3A7
		õ	ILE	74		-19.082	-5.904	1.00	0.00	3A7
ATOM	262							1.00	0.00	3A7
ATOM	263	N	TYR	75 75		-16.900	-6.425			3A7
MOTA	264	CA	TYR	75		-16.765	-6.827	1.00	0.00	
ATOM	265	СВ	TYR	75		-16.348	-8.308	1.00	0.00	3A7
ATOM	266	CG	TYR	75		-17.400	-9.184	1.00	0.00	3A7
ATOM	267	CD1	TYR	75		-17.281	-9.613	1.00	0.00	3A7
ATOM	268	CD2	TYR	75	19.554	-18.513	-9.582	1.00	0.00	3A7
ATOM	269	CE1	TYR	75	16.911	-18.261	-10.415	1.00	0.00	3A7
ATOM	270	CE2	TYR	75	18.983	-19.489	-10.394	1.00	0.00	3A7
ATOM	271	CZ	TYR	75	17.660	-19.367	-10.807	1.00	0.00	3A7
ATOM	272	ОН	TYR	75		-20.361		1.00	0.00	3A7
ATOM	273	c	TYR	75		-15.716	-5.954	1.00	0.00	3A7
ATOM	274	ŏ	TYR	75		-14.543	-6.059	1.00	0.00	3A7
ATOM	275	N	ASP	76		-16.106	-5.059	1.00	0.00	3A7
	276	CA	ASP	76		-15.171	-4.194	1.00	0.00	3A7
ATOM						-15.513	-2.685	1.00	0.00	3A7
ATOM	277	CB	ASP	76 76					0.00	3A7
ATOM	278	CG	ASP	76		-15.259	-2.172	1.00	0.00	3A7
ATOM	279		ASP	76		-15.935	-2.652	1.00	0.00	3A7
MOTA	280		ASP	76		-14.382	-1.279	1.00		3A7
MOTA	281	С	ASP	76		-15.175	-4.597	1.00	0.00	3A7 3A7
ATOM	282	0	ASP	76		-16.000	-4.149	1.00	0.00	3A7 3A7
MOTA	283	N	CYS	77		-14.210	-5.459	1.00	0.00	
MOTA	284	CA	CYS	77		-13.896	-5.902	1.00	0.00	3A7
ATOM	285	CB	CYS	77		-13.074	-4.858	1.00	0.00	3A7
ATOM	286	SG	CYS	77		-13.854	-3.237	1.00	0.00	3A7
ATOM	287	С	CYS	7 <b>7</b>		-15.056	-6.442	1.00	0.00	3A7
ATOM	288	0	CYS	77		-15.442	-5.879	1.00	0.00	3A7
ATOM	289	N	GLN	78	•	-15.613	-7.583	1.00	0.00	3A7
MOTA	290	CA	GLN	78		-16.622	-8.369	1.00	0.00	3A7
ATOM	291	CB	GLN	78	27.325	-16.549	-8.440	1.00	0.00	3A7
ATOM	292	CG	GLN	78	27.848	-15.222	-9.017	1.00	0.00	3A7
ATOM	293	CD	GLN	78	29.378	-15.274	-9.063	1.00	0.00	3A7
ATOM	294	OE1	GLN	78	29.961	-16.057	-9.823	1.00	0.00	3A7
ATOM	295	NE2	GLN	78	30.031	-14.415	-8.222	1.00	0.00	3A7
ATOM	296	С	GLN	78		-18.037	-8.023	1.00	0.00	`3A7
ATOM	297	ō	GLN	78		-18.949	-8.771	1.00	0.00	3A7
ATOM	298	N	GLN	79		-18.277	-6.903	1.00	0.00	3A7
ATOM	299		GLN	79		-19.620	-6.516	1.00	0.00	3A7
				79		-19.978	-5.085	1.00	0.00	3A7
ATOM	300	CB	GLN			-19.895	-4.897	1.00	0.00	3A7
MOTA	301	CG	GLN	79 70				1.00	0.00	3A7
ATOM	302	CD	GLN	79 70		-20.276 -19.589	-3.453 -2.508	1.00	0.00	3A7
ATOM	303		GLN	79 70					0.00	3A7
ATOM	304		GLN	79		-21.399		1.00		3A7
MOTA	305	С	GLN	79		-19.774	-6.615	1.00	0.00	
MOTA	306	0	GLN	79		-18.847	-6.260	1.00	0.00	3A7
ATOM	307	N	PRO	80		-20.926		1.00	0.00	3A7
ATOM	308	CA	PRO	80		-21.225		1.00	0.00	3A7
MOTA	309	CD	PRO	80		-21.867		1.00	0.00	3A7
ATOM	310	СВ	PRO	80		-22.191		1.00	0.00	3A7
MOTA	311	CG	PRO	80	21.950	-22.915	-8.360	1.00	0.00	3A7
ATOM	312	С	PRO	80	20.502	-21.899	-5.737	1.00	0.00	3A7
ATOM	313	0	PRO	80	21.269	-22.746	-5.277	1.00	0.00	3A7
ATOM	314	N	MET	81		-21.571		1.00	0.00	3A7
ATOM	315	ÇA	MET	81		-22.233		1.00	0.00	3A7
ATOM	316	СВ	MET	81		-21.392		1.00	0.00	3A7
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ATOM	317	CG	MET	81	20.582	-21.043	-2.428	1.00	0.00	3A7
ATOM	318	SD	MET	81	20.947		-0.854	1.00	0.00	3A7
MOTA	319	CE	MET	81		-18.650	-1.276	1.00	0.00	3A7 3A7
ATOM	320	c	MET	81 81		-22.487 -21.572	-4.177 -4.447	1.00	0.00	3A7
ATOM ATOM	321 322	о И	MET	82		-23.763	-4.052	1.00	0.00	3A7
ATOM	323	CA	LEU	82		-24.130	-4.201	1.00	0.00	3A7
ATOM	324	СВ	LEU	82		-25.434	-4.990	1.00	0.00	3A7
ATOM	325	CG	LEU	82		-25.122	-6.509	1.00	0.00	3A7
MOTA	326		TEO .	82		-25.569	-7.137	1.00	0.00	3A7 3A7
ATOM	327	CD2		82		-25.622 -24.179	-7.300 -2.843	1.00	0.00 0.00	3A7
ATOM	328 329	С 0	LEU	82 82		-24.903	-1.947	1.00	0.00	3A7
ATOM ATOM	330	N	ALA	83		-23.351	-2.673	1.00	0.00	3A7
ATOM	331	CA	ALA	83	13.243	-23.210	-1.443	1.00	0.00	3A7
MOTA	332	CB	ALA	83		-21.792	-1.267	1.00	0.00	3A7
MOTA	333	С	ALA	83		-24.096	-1.430	1.00	0.00	3A7 3A7
MOTA	334	0	ALA	83		-24.025 -24.967	-2.320 -0.399	1.00	0.00	3A7
ATOM	335 336	N CA	ILE	84 84		-25.985	-0.290	1.00	0.00	3A7
ATOM ATOM	337	СВ	ILE	84		-27.364	0.009	1.00	0.00	3A7
ATOM	338		ILE	84		-28.307	0.374	1.00	0.00	3A7
ATOM	339	CG1	ILE	84		-28.016	-1.243	1.00	0.00	3A7
MOTA	340	CD	ILE	84		-27.201	-2.013	1.00	0.00	3A7 3A7
	341	C	ILE	84		-25.576	0.802 1.921	1.00	0.00	3A7
ATOM	342 343	O N	ILE Thr	84 85		-25.289 -25.597	0.509	1.00	0.00	3A7
MOTA MOTA	344	CA	THR	85		-25.139	1.413	1.00	0.00	3A7
ATOM	345	СВ	THR	85		-23.819	0.999	1.00	0.00	3A7
ATOM	346	OG1	THR	85		-23.627	-0.412	1.00	0.00	3A7
MOTA	347		THR	85		-22.782	1.725	1.00	0.00	3A7 3A7
ATOM	348	C	THR	85		-26.125 -26.730	1.486 0.619	1.00	0.00	3A7
MOTA MOTA	349 350	O N	THR ASP	85 86		-26.396	2.502	1.00	0.00	3A7
ATOM	351	CA	ASP	86		-27.263	2.510	1.00	0.00	3A7
ATOM .	352	СВ	ASP	86	3.722	-27.421	1.361	1.00	0.00	3A7
ATOM	353	CG	ASP	86		-26.055	0.952	1.00	0.00	3A7
ATOM	354		ASP	86		-25.362	1.833 -0.246	1.00	0.00 0.00	3A7 3A7
ATOM	355		ASP ASP	86 86		-25.692 -28.602	3.011	1.00	0.00	3A7
ATOM ATOM	356 357	C	ASP	86		-28.994	2.738	1.00	0.00	3A7
ATOM	358	N	PRO	87		-29.324	3.756	1.00	0.00	3A7
ATOM	359	CA	PRO	87		-30.519	4.472	1.00	0.00	3A7
MOTA	360	CD	PRO	87		-28.734	4.388	1.00	0.00	3A7 3A7
ATOM	361	CB	PRO	87 97		-30.942 -29.914	5.276 4.977	1.00	0.00	3A7
MOTA	362 363	CG C	PRO	87 87		-31.641	3.571	1.00	0.00	3A7
MOTA MOTA	364	Ö	PRO	87		-32.375	3.920	1.00	0.00	3A7
ATOM	365	N	ASP	88	4.533	-31.800	2.413	1.00	0.00	3A7
MOTA	366	CA	ASP	88		-32.846	1.455	1.00	0.00	3A7
ATOM	367	CB <sup>r</sup>	ASP	88		-32.701	0.270	1.00	0.00	3A7 3A7
ATOM	368	CG	ASP	88 88		-32.826 -33.640	0.749 1.676	1.00	0.00	3A7
ATOM ATOM	369 370		ASP ASP	88	_	-32.094	0.198	1.00	0.00	3A7
ATOM	371	c	ASP	88		-32.787	0.909	1.00	0.00	3A7
ATOM	372	0	ASP	88		-33.798	0.830	1.00	0.00	3A7
MOTA	373	N	MET	89		-31.588	0.554	1.00	0.00	3A7 3A7
MOTA	374	CA	MET	89		-31.388	0.009 -0.773	1.00	0.00	3A7
ATOM ATOM	375 376	CB CG	MET MET	89 89		-30.073 -30.035	-1.918	1.00	0.00	3A7
MOTA	377	SD	MET	89		-28.663	-1.731	1.00	0.00	3A7
ATOM	378	CE	MET	89	7.247	-27.425	-1.755	1.00	0.00	3A7
ATOM	379	С	MET	89		-31.390	1.081	1.00	0.00	3A7
ATOM	380	0	MET	89		-31.936	0.893	1.00	0.00	3A7 3A7
ATOM	381	N	ILE	90		-30.824 -30.812	2.267 3.398	1.00	0.00	3A7 3A7
ATOM ATOM	382 383	CA CB	ILE	90 90		-29.908	4.501	1.00		3A7
ATOM	384		ILE	90		-30.036	5.807	1.00		3A7
ATOM	385		ILE	90		-28.467	3.973	1.00	0.00	3A7
ATOM	386	CD	ILE	90		-27.853	3.815	1.00		3A7
ATOM	387	C	ILE	90		-32.218	3.920	1.00		3A7 3A7
MOTA	388	0	ILE	90	11.016	-32.588	4.248	1.00	0.00	3A7

ATOM	389	N	LYS	91	8.877	-33.100	3.925	1.00	0.00	3A7
MOTA	390	CA	LYS	91		-34.479	4.328	1.00	0.00	3A7
ATOM	391 _	СВ	LYS	91		-35.240	4.361	1.00	0.00	3A7
ATOM	392	CG	LYS	91		-36.619	5.036	1.00	0.00	3A7
ATOM	393	CD	LYS	91		-37.269	5.192	1.00	0.00	3A7 3A7
ATOM	394	CE	LYS	91		-38.628 -39.206	5.898 6.031	1.00	0.00	3A7
ATOM	395	NZ	LYS LYS	91 91		-35.200	3.414	1.00	0.00	3A7
ATOM ATOM	396 397	С 0	LYS	91		-36.021	3.838	1.00	0.00	3A7
ATOM	398	N	THR	92		-34.861	2.113	1.00	0.00	3A7
ATOM	399	CA	THR	92		-35.382	1.113	1.00	0.00	3A7
ATOM	400	СВ	THR	92		-34.980	-0.272	1.00	0.00	3A7
ATOM	401		THR	92		-35.206	-0.430	1.00	0.00	3A7
ATOM	402	CG2	THR	92	11.180	-35.836	-1.323	1.00	0.00	3A7
ATOM	403	С	THR	92		-34.904	1.326	1.00	0.00	3A7
MOTA	404	0	THR	92		-35.657	1.196	1.00	0.00	3A7
MOTA	405	N	VAL	93		-33.620	1.730	1.00	0.00	3A7
MOTA	406	CA	VAL	93		-33.006	1.938	1.00	0.00	3A7 3A7
ATOM	407	CB	VAL	93		-31.500	2.127	1.00	0.00	3A7
ATOM	408		VAL	93		-30.752 -31.074	1.061 3.585	1.00	0.00	3A7
ATOM	409 410	CGZ	VAL VAL	93 93		-33.705	3.034	1.00	0.00	3A7
MOTA MOTA	411	0	VAL	93		-33.627	3.002	1.00	0.00	3A7
ATOM	412	N	LEU	94		-34.522	3.946	1.00	0.00	3A7
MOTA	413	CA	LEU	94		-35.450	4.889	1.00	0.00	3A7
ATOM	414	СВ	LEU	94		-36.540	5.429	1.00	0.00	3A7
ATOM	415	CG	LEU	94	12.454	-36.028	6.397	1.00	0.00	3A7
ATOM	416	CD1	LEU	94	11.435	-37.136	6.726	1.00	0.00	3A7
ATOM	417	CD2	LEU	94		-35.489	7.687	1.00	0.00	3A7
MOTA	418	С	LEU	94		-36.253	4.325	1.00	0.00	3A7
ATOM	419	0	LEU	94		-36.171	4.842	1.00	0.00	3A7
ATOM	420	N	VAL	95		-37.041	3.249	1.00	0.00	3A7
ATOM	421	CA	VAL	95		-37.904	2.446	1.00	0.00	3A7 3A7
ATOM	422 423	CB	VAL	95 95		-37.147 -36.331	1.449 2.088	1.00	0.00	3A7
ATOM ATOM	423		VAL VAL	95 95		-38.131	0.379	1.00	0.00	3A7
ATOM	425	C	VAL	95		-38.932	3.269	1.00	0.00	3A7
ATOM	426	ŏ	VAL	95		-38.606	4.052	1.00	0.00	3A7
ATOM	427	N	LYS	96		-40.226	3.099	1.00	0.00	3A7
ATOM	428	CA	LYS	96		-41.310	3.864	1.00	0.00	3A7
ATOM	429	CB	LYS	96	16.284	-41.757	5.021	1.00	0.00	3A7
ATOM	430	CG	LYS	96		-42.863	5.922	1.00	0.00	3A7
ATOM	431	CD .	LYS	96		-43.296	7.055	1.00	0.00	3A7
ATOM	432	CE	LYS	96		-42.211	8.105	1.00	0.00	3A7
ATOM	433	NZ	LYS	96		-41.808	8.783	1.00	0.00	3A7
ATOM	434	C	LYS	96		-42.463	2.917	1.00	0.00	3A7 3A7
ATOM	435	0	LYS	96		-42.998	2.397 2.649	1.00	0.00	3A7
ATOM	436 437	N CA	GLU GLU	97 97		-42.930 -42.451	3.016	1.00	0.00	3A7
ATOM ATOM	438	CB	GLU	97		-41.024	2.498	1.00	0.00	3A7
ATOM	439	CG	GLU	97		-40.894	0.966	1.00	0.00	3A7
ATOM	440	CD	GLU	97		-41.763	0.314	1.00	0.00	3A7
ATOM	441		GLU	97		-42.695	-0.447	1.00	0.00	3A7
ATOM	442		GLU	97		-41.504	0.567	1.00	0.00	3A7
ATOM	443	С	GLU	97	20.318	-42.531	4.499	1.00	0.00	3A7
ATOM	444	0	GLU	97	20.158	-41.560	5.238	1.00	0.00	3A7
ATOM	445	N	CYS	98		-43.711	4.956	1.00	0.00	3A7
MOTA	446	CA	CYS	98		-43.956	6.327	1.00	0.00	3A7
MOTA	447	СВ	CYS	98		-45.456	6.703	1.00	0.00	3A7
ATOM	448	SG	CYS	98		-46.111	6.530	1.00	0.00	3A7 3A7
ATOM	449	C	CYS	98		-43.454 -43.131	6.538		0.00	3A7
ATOM ATOM	450 451	O N	CYS	98 99		-43.131 -43.358	7.656 5.423	1.00	0.00	3A7
ATOM	452	N CA	TYR TYR	99		-43.336	5.352	1.00	0.00	3A7
ATOM	453	CB	TYR	99		-43.602	4.775	1.00	0.00	3A7
ATOM	454	CG	TYR	99		-44.708	5.749	1.00	0.00	3A7
ATON	455		TYR	99		-45.981	5.553	1.00	0.00	3A7
ATOM	456		TYR	99		-44.471	6.875	1.00	0.00	3A7
ATOM	457		TYR	99		-47.000	6.470	1.00	0.00	3A7
ATOM	458	CE2	TYR	99		-45.488	7.791	1.00	0.00	3A7
ATOM	459	CZ	TYR	99		-46.754	7.591	1.00	0.00	3A7
MOTA	460	OH	TYR	99	26.807	-47.785	8.524	1.00	0.00	3A7

ATOM	461	С	TYR	99	24.459 -41.520	4.445	1.00	0.00	3A7
MOTA	462	0	TYR	99	24.717 -41.584	3.244	1.00	0.00	3A7
MOTA	463	N	SER	100	23.943 -40.407	5.029	1.00	0.00	3A7
MOTA	464	CA	SER	100	23.548 -39.211	4.317 4.990	1.00	0.00	3A7 3A7
MOTA	465	CB	SER SER	100 100	22.340 -38.501 22.547 -38.275	6.381	1.00	0.00	3A7
ATOM ATOM	466 467	og C	SER	100	24.721 -38.267	4.207	1.00	0.00	3A7
ATOM	468	ŏ	SER	100	25.295 -37.848	5.211	1.00	0.00	3A7
ATOM	469	N	VAL	101	25.093 -37.923	2.947	1.00	0.00	3A7
ATOM	470	CA	VAL	101	26.233 -37.096	2.616	1.00	0.00	3A7
MOTA	471	CB	VAL	101	26.925 -37.529	1.327	1.00	0.00	3A7 3A7
MOTA	472		VAL	101	28.244 -36.746	1.143 1.394	1.00	0.00 0.00	3A7
ATOM	473 474	CG2 C	VAL VAL	101 101	27.188 -39.049 25.777 -35.663	2.512	1.00	0.00	3A7
ATOM ATOM	475	ŏ	VAL	101	25.384 -35.187	1.447	1.00	0.00	3A7
ATOM	476	N	PHE	102	25.851 -34.944	3.658	1.00	0.00	3A7
ATOM	477	CA	PHE	102	25.588 -33.531	3.774	1.00	0.00	3A7
MOTA	478	CB	PHE	102	24.757 -33.208	5.051	1.00	0.00	3A7 3A7
ATOM	479	CG	PHE	102	24.515 -31.734	5.284 4.236	1.00	0.00	3A7
ATOM	480		PHE	102 102	24.224 -30.854 24.602 -31.227	6.582	1.00	0.00	3A7
ATOM ATOM	481 482		PHE	102	24.063 -29.493	4.481	1.00	0.00	3A7
ATOM	483		PHE	102	24.424 -29.870	6.830	1.00	0.00	3A7
ATOM	484	CZ	PHE	102	24.163 -29.000	5.777	1.00	0.00	3A7
ATOM	485	C	PHE	102	26.945 -32.887	3.838	1.00	0.00	3A7
ATOM	486	0	PHE	102	27.728 -33.174	4.741	1.00	0.00	3A7 3A7
ATOM	487	N	THR	103	27.238 -31.980 28.502 -31.281	2.869 2.757	1.00	0.00	3A7
ATOM ATOM	488 489	CA CB	THR THR	103 103	28.814 -30.904	1.308	1.00	0.00	3A7
ATOM	490		THR	103	30.168 -30.496	1.135	1.00	0.00	3A7
ATOM	491		THR	103	27.858 -29.816	0.779	1.00	0.00	3A7
ATOM	492	С	THR	103	28.484 -30.083	3.685	1.00	0.00	3A7
MOTA	493	0	THR	103	27.430 -29.672	4.169	1.00	0.00	3A7 3A7
ATOM	494	N	ASN	104	29.682 -29.507 29.888 -28.430	3.955 4.899	1.00	0.00 0.00	3A7
ATOM ATOM	495 496	CA CB	ASN ASN	104 104	31.378 -28.320	5.343	1.00	0.00	3A7
ATOM	497	CG	ASN	104	32.353 -28.168	4.161	1.00	0.00	3A7
ATOM	498		ASN	104	32.706 -27.047	3.775	1.00	0.00	3A7
ATOM	499	ND2	ASN	104	32.796 -29.333	3.597	1.00	0.00	3A7
ATOM	500	С	ASN	104	29.418 -27.105	4.342	1.00	0.00	3A7 3A7
ATOM	501	.0	ASN.	104	29.471 -26.868 28.961 -26.205	3.135 5.250	1.00	0.00	3A7
ATOM ATOM	502 503	N CA	ARG ARG	105 105	28.538 -24.859	4.929	1.00	0.00	3A7
ATOM	504	CB	ARG	105	27.556 -24.275	5.967	1.00	0.00	3A7
ATOM	505	CG	ARG	105	26.214 -25.018	6.037	1.00	0.00	3A7
ATOM	506	CD	ARG	105	25.300 -24.418	7.111	1.00	0.00	3A7
ATOM	507	NE	ARG	105	24.029 -25.205	7.173	1.00	0.00	3A7 3A7
ATOM	508	CZ	ARG ARG	105 105	23.007 -24.845 21.860 -25.583	8.007 8.027	1.00	0.00 0.00	3A7
ATOM . ATOM	509 510		ARG	105	23.124 -23.752	8.816	1.00	0.00	3A7
ATOM	511	c	ARG	105	29.756 -23.977	4.884	1.00	0.00	3A7
ATOM	512	0	ARG	105	30.703 -24.170	5.645	1.00	0.00	3A7
ATOM	513	N	ARG	106	29.750 -22.991	3.955	1.00	0.00	3A7
ATOM	514	CA	ARG	106	30.909 -22.177	3.639	1.00	0.00	3A7 3A7
ATOM	515	CB CG	ARG ARG	106 106	30.852 -21.586 30.675 -22.664	2.205 1.121	1.00	0.00	3A7
ATOM ATOM	516 517	CD	ARG	106	30.504 -22.088	-0.292	1.00	0.00	3A7
ATOM	518	NE	ARG	106	31.739 -21.318	-0.652	1.00	0.00	3A7
ATOM	519	CZ	ARG	106	31.841 -20.619	-1.824	1.00	0.00	3A7
ATOM	520		ARG	106	32.985 -19.927	-2.100	1.00	0.00	3A7
ATOM	521		ARG	106	30.809 -20.607	-2.718	1.00	0.00	3A7 3A7
MOTA	522	C	ARG	106 106	31.190 -21.087 32.357 -20.971	4.647 5.015	1.00	0.00 0.00	3A7
MOTA MOTA	523 524	O N	ARG PRO	107	30.250 -20.287	5.178	1.00	0.00	3A7
ATOM	525	CA	PRO	107	30.565 -19.212	6.105	1.00	0.00 -	
ATOM	526	CD	PRO	107	28.890 -20.159	4.663	1.00	0.00	3A7
ATOM	527	CB	PRO	107	29.245 -18.456	6.287	1.00	0.00	3A7
ATOM	528	CG	PRO	107	28.480 -18.724	4.991	1.00	0.00	3A7 3A7
ATOM	529	C	PRO	107 107	31.061 -19.732 31.834 -19.045	7.435 8.098	1.00	0.00	3A7
ATOM ATOM	530 531	о И	PRO PHE	107	30.645 -20.949	7.846	1.00	0.00	3A7
ATOM	532	CA	PHE	108	30.989 -21.534	9.116	1.00	0.00	3A7

ATOM	533	СВ	PHE	108	29.984	-22.623	9.543	1.00	0.00	3A7
MOTA	534	CG	PHE	108		-22.099	9.639	1.00	0.00	3A7
MOTA	535 536		PHE	108 108		-21.852 -21.924	8.488 10.885	1.00	0.00	3A7 3A7
ATOM ATOM	537		PHE	108		-21.446	8.575	1.00	0.00	3A7
MOTA	538		PHE	108		-21.528	10.976	1.00	0.00	3A7
MOTA	539	CZ	PHE	108		-21.298	9.821	1.00	0.00	3A7
MOTA	540	С	PHE	108		-22.153	9.070	1.00	0.00	3A7
MOTA	541	0	PHE	108		-22.269	10.095	1.00	0.00	3A7 3A7
MOTA	542 543	N CA	GLY	109 109		-22.555 -23.135	7.875 7.691	1.00	0.00	3A7 3A7
ATOM ATOM	544	C	GLY	109		-22.254	8.056	1.00	0.00	3A7
ATOM	545	ō	GLY	109		-22.774	8.561	1.00	0.00	3A7
ATOM	546	N	PRO	110		-20.938	7.853	1.00	0.00	3A7
ATOM	547	CA	PRO	110		-20.023	8.270	1.00	0.00	3A7
ATOM	548	CD	PRO	110		-20.430	6.620	1.00	0.00	3A7 3A7
ATOM ATOM	549 550	CB	PRO PRO	110 110		-18.682 -19.054	7.743 6.361	1.00	0.00	3A7
ATOM	551	č	PRO	110		-19.895	9.765	1.00	0.00	3A7
ATOM	552	o	PRO	110		-19.525	10.094	1.00	0.00	3A7
ATOM	553	N	VAL	111		-20.153	10.690	1.00	0.00	3A7
ATOM	554	CA	VAL	111		-19.847	12.107	1.00	0.00	3A7
ATOM	555 556	CB	VAL	111 111		-19.678 -18.645	12.890 12.147	1.00	0.00	3A7 3A7
ATOM ATOM	557		VAL	111		-21.007	13.118	1.00	0.00	3A7
ATOM	558	c	VAL	111		-20.855	12.787	1.00	0.00	3A7
ATOM	559	0	VAL	111		-22.067	12.658	1.00	0.00	3A7
ATOM	560	N	GLY	112		-20.325	13.502	1.00	0.00	3A7
ATOM	561	CA	GLY	112		-21.102	14.130	1.00	0.00	· 3A7
ATOM ATOM	562 563	С 0	GLY	112 112		-20.384 -19.155	13.863 13.891	1.00	0.00	3A7
ATOM	564	N	PHE	113		-21.162	13.582	1.00	0.00	3A7
ATOM	565	CA	PHE	113	42.395	-20.640	13.182	1.00	0.00	3A7
MOTA	566	CB	PHE	113		-20.476	14.380	1.00	0.00	3A7
ATOM	567	CG	PHE	113		-19.854	13.980	1.00	0.00	3A7 3A7
ATOM ATOM	568 569		PHE	113		-20.468 -18.671	14.346 13.239	1.00	0.00	3A7 3A7
ATOM	570		PHE	113		-19.918	13.233	1.00	0.00	3A7
ATOM	571		PHE	113		-18.120	12.861	1.00	0.00	3A7
MOTA	572	CZ	PHE	113		-18.744	13.226	1.00	0.00	3A7
MOTA	573	C	PHE	113		-21.648	12.181	1.00	0.00	3A7
ATOM ATOM	574 575	O N	PHE	113 114		-22.372 -21.708	12.431 11.011	1.00	0.00	· 3A7 3A7
ATOM	576	CA	MET	114		-22.600	9.882	1.00	0.00	3A7
ATOM	577	CB	MET	114		-22.624	9.331	1.00	0.00	3A7
MOTA	578	ÇG	MET	114		-21.313	8.647	1.00	0.00	3A7
ATOM	579	SD	MET	114		-19.936	9.761	1.00	0.00	3A7
ATOM	580 501	CE	MET	114		-18.779 -24.012	8.440 10.217	1.00	0.00	3A7 3A7
ATOM ATOM	581 582	С О	MET MET	114 . 114		-24.294	11.346	1.00	0.00	3A7
ATOM	583	N	LYS	115		-24.924	9.208	1.00	0.00	3A7
ATOM	584	CA	LYS	115		-26.343	9.268	1.00	0.00	3A7
ATOM	585	СВ	LYS	115		-27.158	10.423	1.00	0.00	3A7
ATOM	586	CG	LYS	115		-27.432 -26.252	10.251 10.533	1.00	0.00	3A7 3A7
ATOM ATOM	587 588	CD CE	LYS LYS	115 115		-25.758	11.988	1.00	0.00	3A7
ATOM	589	NZ	LYS	115		-26.832	12.922	1.00	0.00	3A7
MOTA	590	С	LYS	115	40.202	-26.569	9.300	1.00	0.00	3 <b>A</b> 7
ATOM	591	0	LYS	115		-26.979	8.297	1.00	0.00	3A7
ATOM	592	N	ASN	116		-26.341 -26.560	10.491 10.889	1.00	0.00	3A7 3A7
ATOM ATOM	593 594	CA CB	ASN ASN	116 116		-25.724	10.889	1.00	0.00	3A7
ATOM	595	CG	ASN	116		-26.079	8.657	1.00	0.00	3A7
ATOM	596	OD1		116	37.384	-25.453	7.745	1.00	0.00	3A7
ATOM	597	ND2		116		-27.074	8.437	1.00	0.00	3A7
ATOM	598	C	ASN	116		-28.039	10.949	1.00	0.00	3A7
ATOM ATOM	599 600	O N	ASN ALA	116 117		-28.777 -28.501	9.979 12.134	1.00	0.00	3A7 3A7
ATOM	601	CA	ALA	117		-29.900	12.415	1.00	0.00	3A7
ATOM	602	СВ	ALA	117		-30.247	13.899	1.00	0.00	3A7
MOTA	603	C	ALA	117		-30.294	12.024	1.00	0.00	3A7
ATOM	604	0	ALA	117	35.542	-30.857	10.951	1.00	0.00	3A7

ATOM	605	N	ILE	118	34.758	-30.027	12.909	1.00	0.00	3A7
ATOM	606	CA	ILE	118	33.403	-30.498	12.732	1.00	0.00	3A7
MOTA	607	CB	ILE	118		-31.666	13.661	1.00	0.00	3A7
ATOM	608		ILE	118		-32.948	13.008	1.00	0.00	3A7
ATOM ATOM	609 610	CD	ILE ILE	118 118		-31.523 -30.511	15.097 15.983	1.00	0.00 0.00	3A7 3A7
ATOM	611	c	ILE	118		-29.333	12.894	1.00	0.00	3A7
ATOM	612	ō	ILE	118		-29.399	13.643	1.00	0.00	3A7
ATOM	613	N	SER	119		-28.231	12.139	1.00	0.00	3A7
MOTA	614	CA	SER	119		-27.054	12.114	1.00	0.00	3A7
ATOM	615	CB	SER	119		-25.747	11.972	1.00	0.00	3A7
ATOM ATOM	616 617	OG C	SER SER	119 119		-25.595 -27.178	13.079 10.949	1.00	0.00 0.00	3A7 3A7
ATOM	618	ò	SER	119		-26.507	9.930	1.00	0.00	3A7
ATOM	619	N	ILE	120		-28.096	11.093	1.00	0.00	3A7
ATOM	620	CA	ILE	120	28.963	-28.576	10.086	1.00	0.00	3A7
ATOM	621	CB	ILE	120		-27.497	9.294	1.00	0.00	3A7
ATOM	622		ILE	120		-28.166	8.349	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	623 624	CD	ILE ILE	120 120		-26.482 -27.096	10.237 11.166	1.00	0.00	3A7
ATOM	625	c	ILE	120		-29.507	9.171	1.00	0.00	3A7
ATOM	626	ō	ILE	120		-29.081	8.276	1.00	0.00	3A7
ATOM	627	N	ALA	121		-30.825	9.421	1.00	0.00	3A7
ATOM	628	CA	ALA	121		-31.779	8.845	1.00	0.00	3A7
ATOM	629	СВ	ALA	121		-32.322	9.891	1.00	0.00	3A7 3A7
ATOM ATOM	630 631	С 0	ALA ALA	121 121		-32.895 -33.051	8.190 8.369	1.00	0.00 0.00	3A7
ATOM	632	N	GLU	122		-33.699	7.384	1.00	0.00	3A7
ATOM	633	CA	GLU	122	30.006	-34.785	6.580	1.00	0.00	3A7
ATOM	634	СВ	GLU	122		-34.988	5.292	1.00	0.00	3A7
ATOM	635	CG	GLU	122		-33.676	4.532	1.00	0.00	3A7
ATOM	636	CD	GLU	122 122		-33.979 -34.679	3.190 2.360	1.00	0.00	3A7 3A7
ATOM ATOM	637 638		GLU GLU	122		-33.510	2.975	1.00	0.00	3A7
ATOM	639	c	GLU	122		-36.057	7.368	1.00	0.00	3A7
MOTA	640	0	GLU	122		-36.091	8.393	1.00	0.00	3A7
MOTA	641	N	ASP	123		-37.130	6.889	1.00	0.00	3A7
ATOM	642	CA	ASP	123		-38.402	7.576	1.00	0.00	3A7 3A7
ATOM ATOM	643 644	CB CG	ASP ASP	123 123		-39.195 -39.602	7.107 5.628	1.00	0.00	3A7 3A7
ATOM	645		ASP	123		-38.707	4.763	1.00	0.00	3A7
ATOM	646		ASP	123		-40.822	5.354	1.00	0.00	3A7
ATOM	647	С	ASP	123		~39.259	7.471	1.00	0.00	3A7
ATOM	648	0	ASP	123		-39.955	6.485	1.00	0.00	3A7
ATOM ATOM	649 650	N CA	GLU	124 124		-39.189 -39.870	8.540 8.683	1.00	0.00	3A7 3A7
ATOM	651	СВ	GLU	124		-39.519	7.609	1.00	0.00	3A7
ATOM	652	CG	GLU	124		-40.257	7.793	1.00	0.00	3A7
ATOM	653	CD	GLU.	124		-39.851	6.672	1.00	0.00	3A7
ATOM	654		GLU	124		-39.275	6.989	1.00	0.00	3A7
ATOM	655	OE2	GLU	124		-40.115 -39.381	5.486 10.020	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	656 657	С 0	GTN GTN	124 124		-40.149	10.020	1.00	0.00	3A7
ATOM	658	N	GLU	125		-38.047	10.219	1.00	0.00	3A7
ATOM	659	CA	GLU	125		-37.358	11.455	1.00	0.00	3A7
ATOM	660	СВ	GLU	125		-36.078	11.267	1.00	0.00	3A7
ATOM	661	CG	GLU	125		-36.303	10.505	1.00	0.00	3A7
MOTA MOTA	662 663	CD	GLU	125 125		-37.314 -38.392	11.254 10.667	1.00	0.00 0.00	3A7 3A7
ATOM	664		GLU	125		-37.024	12.418	1.00	0.00	3A7
ATOM	665	C	GLU	125		-36.969	12.096	1.00	0.00	3A7
ATOM	666	0	GLU	125		-36.775	13.306	1.00	0.00	3A7
ATOM	667	N	TRP	126		-36.843	11.315	1.00	0.00	3A7
ATOM ATOM	668	CA CB	TRP	126 126		-36.458 -36.001	11.855 10.762	1.00	0.00 0.00	3A7 3A7
ATOM	669 670	CG	TRP TRP	126		-34.955	11.159	1.00	0.00	3A7
ATOM	671	CD2		126		-33.684	11.776	1.00	0.00	3A7
ATOM	672	CD1		126	26.092	-34.933	10.869	1.00	0.00	3A7
ATOM	673	NE1		126		-33.741	11.271	1.00	0.00	3A7
ATOM	674	CE2		126		-32.954	11.818	1.00	0.00	3A7
ATOM ATOM	675 676	CE3		126 126		-33.139 -31.670	12.252 12.329	1.00	0.00 0.00	3A7 3A7
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ATOM	677	CZ3	TRP	126		28.868	-31.850	12.774	1.00	0.00	3A7
MOTA	678		TRP	126		27.680	-31.123	12.810	1.00	0.00	3A7
ATOM	679	С	TRP	126		28.874	-37.602	12.636	1.00	0.00	3A7
ATOM	680	0	TRP	126			-37.423	13.750	1.00	0.00	3A7
MOTA	681	N	LYS	127			-38.842	12.090	1.00	0.00	3A7
ATOM	682	CA	LYS	127			-40.060	12.743	1.00	0.00	3A7
ATOM	683	СВ	LYS	127			-41.279	11.833	1.00	0.00	3A7 3A7
ATOM	684	CG	LYS	127			-42.581	12.315 11.316	1.00	0.00	3A7
MOTA	685	CD	LYS	127			-43.736 -45.046	11.770	1.00	0.00	3A7
ATOM ATOM	686 687	CE NZ	LYS LYS	127 127			-44.893	11.883	1.00	0.00	3A7
ATOM	688	C	LYS	127			-40.320	14.072	1.00	0.00	3A7
ATOM	689	ŏ	LYS	127			-40.651	15.070	1.00	0.00	3A7
ATOM	690	N	ARG	128			-40.112	14.123	1.00	0.00	3A7
ATOM	691	CA	ARG	128		31.301	-40.271	15.331	1.00	0.00	3A7
ATOM	692	СВ	ARG	128		32.812	-40.274	15.061	1.00	0.00	3A7
ATOM	693	CG	ARG	128		33.252	~41.515	14.267	1.00	0.00	3A7
ATOM	694	CD	ARG	128		34.765	-41.777	14.317	1.00	0.00	3A7
MOTA	695	NE	ARG	128			-41.942	15.749	1.00	0.00	3A7
MOTA	696	CZ	ARG	128			-43.090	16.469	1.00	0.00	3A7
ATOM	697		ARG	128			-43.140	17.776	1.00	0.00	3A7 3A7
ATOM	698		ARG	128			-44.186	15.894	1.00	0.00	3A7
ATOM	699	C	ARG	128			-39.217	16.367 17.535	1.00	0.00	. 3A7
MOTA	700	0	ARG	128 129			-39.549 -37.931	15.976	1.00	0.00	3A7
ATOM ATOM	701 702	· CA	ILE	129			-36.852	16.897	1.00	0.00	3A7
ATOM	703	СВ	ILE	129			-35.498	16.229	1.00	0.00	3A7
ATOM	704		ILE	129			-34.398	16.740	1.00	0.00	3A7
ATOM	705		ILE	129			-34.975	16.405	1.00	0.00	3A7
ATOM	706	CD	ILE	129		33.250	-35.944	16.093	1.00	0.00	3A7
ATOM	707	С	ILE	129		29.095	-37.028	17.444	1.00	0.00	3A7
MOTA	708	0	ILE	129			-36.896	18.640	1.00	0.00	3A7
ATOM	709	N	ARG	130			-37.398	16.595	1.00	0.00	3A7
ATOM	710	CA	ARG	130			-37.661	17.021	1.00	0.00	3A7
ATOM	711	CB	ARG	130			-37.943	15.811	1.00	0.00	3A7 3A7
ATOM	.712	CG	ARG	130 130	2 .		-36.681 -36.942	14.987 13.796	1.00	0.00	3A7
ATOM ATOM	713 714	CD NE	ARG	130			-37.896	12.857	1.00	0.00	3A7
ATOM	715	CZ	ARG	130			-38.311	11.694	1.00	0.00	3A7
ATOM	716		ARG	130			-39.169	10.868	1.00	0.00	3A7
ATOM	717		ARG	130			-37.869	11.351	1.00	0.00	. 3A7
ATOM	718	C	ARG	130		26.695	-38.843	17.970	1.00	0.00	3A7
ATOM	719	0	ARG	130		26.037	-38.756	18.996	1.00	0.00	3A7
MOTA	720	N	SER	131			-39.943	17.701	1.00	0.00	3A7
MOTA	721	CA	SER	131			-41.105	18.571	1.00	0.00	3A7
ATOM	722	СВ	SER	131			-42.268	17.985	1.00	0.00	3A7
ATOM	723	OG	SER	131			-41.986	17.760	1.00	0.00	3A7 3A7
ATOM	. 724	C	SER	131			-40.816	19.936	1.00	0.00	3A7
ATOM	725	.0	SER	131			-41,352 -39.936	20.947 19.998	1.00	0.00	. 3A7
ATOM ATOM	726 727	N CA	LEU	132 132			-39.583	21.240	1.00	0.00	3A7
ATOM	728	СВ	LEU	132			-38.838	20.968	1.00	0.00	3A7
ATOM	729	CG	LEU	132			-39.732	20.333	1.00	0.00	3A7
ATOM	730		LEU	132			-38.875	19.583	1.00	0.00	3A7
ATOM	731		LEU	132		32.782	-40.648	21.366	1.00	0.00	3A7
ATOM	732	С	LEU	132			-38.721	22.089	1.00	0.00	3A7
MOTA	733	0	LEU	132			-38.937	23.289	1.00	0.00	3A7
ATOM	734	И	LEU	133			-37.745	21.460	1.00	0.00	3A7
ATOM	735	CA	LEU	133			-36.794	22.145	1.00	0.00	3A7
ATOM	736	CB	LEU	133			-35.547	21.272	1.00	0.00	3A7 3A7
ATOM	737	CG CD1	LEU	133			-34.787 -33.493	20.869 20.117	1.00	0.00	3A7
ATOM ATOM	738 739		LEU	133 133			-33.493	22.052	1.00	0.00	3A7
ATOM	740	CDZ	LEU	133			-37.334	22.547	1.00	0.00	3A7
ATOM	741	Ö	LEU	133			-36.955	23.590	1.00	0.00	3A7
ATOM	742	N	SER	134			-38.237	21.738	1.00	0.00	3A7
ATOM	743	CA	SER	134			-38.748	21.970	1.00	0.00	3A7
ATOM	744	СВ	SER	134			-39.662	20.844	1.00	0.00	
MOTA	745	OG	SER	134			-40.706	20.461	1.00	0.00	3A7
MOTA	746	С	SER	134			-39.430	23.296	1.00	0.00	3A7
MOTA	747	0	SER	134			-39.226	23.854	1.00	0.00	3A7
MOTA	748	Ŋ	PRO	135		24.715	-40.198	23.891	1.00	0.00	3A7

ATOM	749	CA	PRO	135	24.491	-40.773	25.190	1.00	0.00	3A7
MOTA	750	CD	PRO	135	25.854	-40.834	23.260	1.00	0.00	3A7
MOTA	751	CB	PRO	135	25.551	-41.871	25.355	1.00	0.00	
MOTA	752	CG	PRO	135		-42.203	23.924	1.00	0.00	3A7
ATOM	753	С	PRO	135		-39.783	26.310	1.00	0.00	3A7
ATOM	754	0	PRO	135		-39.912	27.273	1.00	0.00	3A7
ATOM	755	N	THR	136		-38.805	26.231	1.00	0.00	3A7 3A7
ATOM	756	CA	THR	136		-37.840	27.291	1.00	0.00	3A7
ATOM	757	CB	THR	136		-37.210	27.207 25.918	1.00	0.00	3A7
ATOM	758 759		THR THR	136 136		-36.654 -38.319	27.492	1.00	0.00	3A7
ATOM ATOM	760	C	THR	136		-36.769	27.320	1.00	0.00	3A7
ATOM	761	ŏ	THR	136		-36.212	28.360	1.00	0.00	3A7
ATOM	762	N	PHE	137		-36.471	26.165	1.00	0.00	3A7
ATOM	763	CA	PHE	137	23.044	-35.454	26.069	1.00	0.00	3A7
ATOM	764	СВ	PHE	137	23.219	-34.665	24.778	1.00	0.00	3A7
ATOM	765	CG	PHE	137	24.305	-33.645	25.018	1.00	0.00	3A7
ATOM	766	CD1	PHE	137		-33.792	24.468	1.00	0.00	3A7
ATOM	767		PHE	137		-32.535	25.831	1.00	0.00	3A7
ATOM	768		PHE	137		-32.863	24.725	1.00	0.00	3A7
ATOM	769		PHE	137		-31.590	26.070	1.00	0.00	3A7
ATOM	770	CZ	PHE	137		-31.757	25.524	1.00	0.00	3A7 3A7
ATOM	771	C	PHE	137		-36.153 -35.799	26.100 25.406	1.00	0.00	3A7
MOTA	772 773	O N	PHE	137 138		-37.179	26.952	1.00	0.00	3A7
ATOM ATOM	774	CA	THR THR	138		-37.782	27.179	1.00	0.00	3A7
ATOM	775	СВ	THR	138		-39.259	27.505	1.00	0.00	3A7
ATOM	776		THR	138		-39.549	28.518	1.00	0.00	3A7
ATOM	777	CG2	THR	138		-40.035	26.226	1.00	0.00	3A7
ATOM	778	С	THR	138	19.588	-37.063	28.326	1.00	0.00	3A7
ATOM	779	0	THR	138		-36.412	29.149	1.00	0.00	3A7
MOTA	780	N	SER	139		-37.211	28.416	1.00	0.00	3A7
ATOM	781	CA	SER	139		-36.585	29.427	1.00	0.00	3A7
ATOM	782	СВ	SER	139		-36.809	29.183	1.00	0.00	3A7
ATOM	783	OG	SER	139		-38.188	29.037	1.00	0.00	3A7 3A7
ATOM	784	C	SER	139 .		-37.053	30.810 31.765	1.00	0.00	3A7
ATOM	785 786	O N	SER GLY	139 140		-36.290 -38.318	30.922	1.00	0.00	3A7
ATOM ATOM	787	CA	GLY	140		-38.898	32.158	1.00	0.00	3A7
ATOM	788	C	GLY	140		-38.362	32.618	1.00	0.00	3A7
ATOM	789	ō	GLY	140		-38.260	33.820	1.00	0.00	3A7
ATOM	790	N	LYS	141	20.933	-38.021	31.673	1.00	0.00	3A7
ATOM	791	CA	LYS	141	22.309	-37.803	32.064	1.00	0.00	3A7
ATOM	792	СВ	LYS	141		-38.611	31.169	1.00	0.00	3A7
ATOM	793	CG	LYS	141		-40.129	31.293	1.00	0.00	3A7
ATOM	794	CD	LYS	141		-40.944	30.571	1.00	0.00	3A7
ATOM	795	CE	LYS	141		-42.456	30.655	1.00	0.00	3A7 3A7
	796	NZ	LYS	141		-43.189 -36.386	29.928 32.232	1.00	0.00	3A7
ATOM . ATOM	797 798	C O	LYS LYS	141 141		-35.680	33.265	1.00	0.00	3A7
ATOM	799	N	LEU	142		-36.031	31.185	1.00	0.00	3A7
ATOM	800	CA	LEU	142		-34.970	31.099	1.00	0.00	3A7
ATOM	801	СВ	LEU	142		-33.593	30.894	1.00	0.00	3A7
ATOM	802	CG	LEU	142	24.455	-32.799	29.656	1.00	0.00	3A7
ATOM	803		LEU	142	23.560	-31.564	29.439	1.00	0.00	3A7
ATOM	804	CD2	LEU	142		-32.407	29.718	1.00	0.00	3A7
ATOM	805	С	LEU	142		-34.903	32.241	1.00	0.00	3A7
ATOM	806	0	LEU	142		-33.901	32.398	1.00	0.00	3A7
ATOM	807	N	LYS	143		-35.975	33.085	1.00	0.00	3A7
ATOM	808	CA	LYS	143		-36.077	34.381	1.00	0.00	3A7 3A7
ATOM	809 810	CB CG	LYS LYS	143 143		-35.966 -37.003	34.315 33.373	1.00	0.00	3A7
ATOM ATOM	811	CD	LYS	143		-38.480	33.573	1.00	0.00	3A7
ATOM	812	CE.	LYS	143		-39.129	34.873	1.00	0.00	3A7
ATOM	813	NZ	LYS	143		-38.601	36.117	1.00	0.00	3A7
ATOM	814	C	LYS	143		-35.060	35.351	1.00	0.00	3A7
ATOM	815	ŏ	LYS	143		-34.248	35.919	1.00	0.00	3A7
ATOM	816	N	GLU	144	24.476	-35.097	35.479	1.00	0.00	3A7
ATOM	817	CA	GLU	144		-34.122	36.090	1.00	0.00	3A7
MOTA	818	СВ	GLU	144		-33.575	37.466	1.00	0.00	3A7
MOTA	819	CG	GLU	144		-34.669	38.535	1.00	0.00	3A7
MOTA	820	CD	GLU.	144	24.730	-34.037	39.820	1.00	0.00	3A7

ATOM	821	OE1	GLU	144	25.849 -34.42	22 40.255	1.00	0.00	3A7
MOTA	822	OE2		144	24.022 -33.10		1.00	0.00	3A7
ATOM	823	C	GLU	144	23.380 -32.9		1.00 1.00	0.00	3A7 3A7
ATOM ATOM	824 825	O N	GLU MET	144 145	24.284 -32.10 22.163 -32.80		1.00	0.00	3A7
ATOM	826	CA	MET	145	21.768 -31.69		1.00	0.00	3A7
ATOM	827	СВ	MET	145	21.203 -31.93		1.00	0.00	3A7
ATOM	828	CG	MET	145	20.243 -33.1		1.00	0.00	3A7
MOTA	829	SD	MET	145	19.496 -33.3		1.00	0.00	3A7 3A7
ATOM	830	CE	MET	145	18.314 -31.9° 20.736 -30.9°		1.00 1.00	0.00	3A7 3A7
ATOM	831 832	С 0	MET MET	145 145	20.810 -29.7		1.00	0.00	3A7
ATOM ATOM	833	N	VAL	146	19.718 -31.6		1.00	0.00	3A7
ATOM	834	CA	VAL	146	18.618 -30.9		1.00	0.00	3A7
MOTA	835	CB	VAL	146	17.494 -31.8		1.00	0.00	3A7
MOTA	836		VAL	146	16.290 -30.9		1.00	0.00	3A7 3A7
ATOM	837		VAL	146	17.145 -32.7 19.066 -30.1		1.00	0.00	3A7
ATOM ATOM	838 839	С 0	VAL VAL	146 146	18.633 -29.0		1.00	0.00	3A7
ATOM	840	N	PRO	147	19.976 -30.6		1.00	0.00	3A7
ATOM	841	CA	PRO	147	20.491 -29.8		1.00	0.00	3A7
ATOM	842	CD	PRO	147	20.305 -32.0		1.00	0.00	3A7
MOTA	843	CB	PRO	147	21.360 -30.8		1.00	0.00 0.00	3A7 3A7
ATOM	844	CG	PRO	147	20.726 -32.2 21.286 -28.6		1.00	0.00	3A7
ATOM ATOM	845 846	С 0	PRO PRO	147 147	21.286 -27.6		1.00	0.00	3A7
ATOM	847	N	ILE	148	21.943 -28.7		1.00	0.00	3A7
ATOM	848	CA	ILE	148	22.723 -27.6		1.00	0.00	3A7
ATOM	849	CB	ILE	148	23.664 -28.1		1.00	0.00	3A7 3A7
ATOM	850		ILE	148	24.341 -26.9		1.00	0.00	3A7
ATOM	851 852	CGI	ILE	148 148	24.796 -29.0 24.460 -30.1		1.00	0.00	3A7
ATOM ATOM	853	C	ILE	148	21.813 -26.5		1.00	0.00	. 3A7
ATOM	854	ō	ILE	148	22.073 -25.3		1.00	0.00	3A7
ATOM	855	N	ILE	149	20.672 -26.9			0.00	3A7
ATOM	856	CA	ILE	149	19.682 -26.0			0.00	3A7 3A7
ATOM	857	CB	ILE	149 149	18.645 -26.7 17.595 -25.7			0.00	3A7
ATOM ATOM	858 859		ILE	149	19.377 -27.3			0.00	3A7
ATOM	860	CD	ILE	149	18.552 -28.4			0.00	3A7
ATOM	861	С	ILE	149	19.032 -25.3			0.00	3A7
MOTA	862	0	ILE	149	18.779 -24.1			0.00	3A7 3A7
ATOM	863	N	ALA	150 150	18.793 -26.0 18.229 -25.4			0.00	3A7
MOTA MOTA	864 865	CA CB	ALA ALA	150	17.894 -26.5			0.00	3A7
ATOM	866	č	ALA	150	19.160 -24.4			0.00	. 3A7
ATOM	867	0	ALA	150	. 18.723 -23.4			0.00	3A7
MOTA	868	N	GLN	151	20.488 -24.7			0.00 0.00	3A7 3A7
ATOM	869	CA	GLN	151 .	21.492 -23.8 22.910 -24.4			0.00	3A7
ATOM ATOM	870 871	CB CG	GLN GLN	151 151	23.192 -25.4			0.00	3A7
ATOM	872	CD	GLN	151	24.551 -26.1			0.00	3A7
ATOM	873		GLN	151	25.580 -25.4	144 40.306		0.00	3A7
ATOM	874		GLN	151	24.541 -27.4			0.00	3A7 3A7
ATOM	875	C	GLN	151	21.475 -22.4 21.418 -21.4			0.00	3A7
ATOM ATOM	876 877	O N	GLN TYR	151 152	21.474 -22.5			0.00	3A7
MOTA	878	CA	TYR	152	21.438 -21.2			0.00	3A7
ATOM	879	СВ	TYR	152	21.651 -21.5			0.00	3A7
MOTA	880	CG	TYR		22.236 -20.2			0.00	3A7 3A7
MOTA	881		TYR	152	23.578 -19.9 21.411 -19.1			0.00	3A7 3A7
MOTA	882 883		TYR TYR	152 152	24.053 -18.3			0.00	3A7
ATOM ATOM	884		TYR	152	21.870 -17.8				3A7
ATOM	885	CZ	TYR		23.208 -17.6	612 35.20	1.00	0.00	3A7
MOTA	886	ОН	TYR	152	23.690 -16.3			0.00	3A7
MOTA	887	C	TYR		20.140 -20.5				3A7 3A7
ATOM	888	0	TYR		20.108 -19.3 19.025 -21.3				3A7
ATOM ATOM	889 890	N CA	GLY GLY	153 153	17.715 -20.				3A7
ATOM	891	C	GLY		17.596 -19.				3A7
MOTA	892	ŏ	GLY		16.977 -18.			0.00	3A7

ATOM	893	N	ASP	154	18.270 -20.45	7 39.650	1.00	0.00	3A7
ATOM	894	CA	ASP	154	18.353 -19.78		1.00	0.00	3A7
MOTA	895	CB	ASP	154	19.017 -20.68		1.00	0.00	3A7
ATOM	896	CG	ASP	154	18.142 -21.90		1.00	0.00	3A7 3A7
ATOM	897		ASP	154	16.975 -21.96 18.643 -22.79		1.00	0.00 0.00	3A7
ATOM	898	OD2 C	ASP ASP	154 154	19.130 -18.48		1.00	0.00	3A7
ATOM ATOM	899 900	o	ASP	154	18.726 -17.46		1.00	0.00	3A7
ATOM	901	N	VAL	155	20.243 -18.47		1.00	0.00	3A7
ATOM	902	CA	VAL	155	21.039 -17.29		1.00	0.00	3A7
ATOM	903	СВ	VAL	155	22.308 -17.63		1.00	0.00	3A7
MOTA	904		VAL	155	23.103 -16.37		1.00	0.00	3A7
ATOM	905		VAL	155	23.251 -18.53		1.00	0.00 0.00	3A7 3A7
ATOM	906	C	VAL	155	20.273 -16.24 20.407 -15.00		1.00	0.00	3A7
ATOM ATOM	907 908	<b>о</b>	VAL LEU	155 156	19.427 -16.65		1.00	0.00	3A7
ATOM	909	CA	LEU	156	18.566 -15.75		1.00	0.00	3A7
ATOM	910	СВ	LEU	156	17.791 -16.49	6 36.208	1.00	0.00	3A7
ATOM	911	CG	LEU	156	17.040 -15.50		1.00	0.00	3A7
ATOM	912		LEU	156	17.539 -15.52		1.00	0.00	3A7 3A7
ATOM	913		LEU	156	15.520 -15.74		1.00	0.00 0.00	. 3A7
ATOM	914	C	LEU	156 156	17.570 -15.04 17.442 -13.83		1.00	0.00	3A7
ATOM ATOM	915 916	O N	LEU VAL	157	16.840 -15.80		1.00	0.00	3A7
ATOM	917	CA	VAL	157	15.830 -15.29		1.00	0.00	3A7
ATOM	918	СВ	VAL	157	15.164 -16.4	19 40.629	1.00	0.00	3A7
ATOM	919		VAL	157	14.204 -15.9		1.00	0.00	3A7
ATOM	920		VAL	157	14.373 -17.2			0.00	3A7 3A7
MOTA	921	C	VAL	157	16.437 -14.33 15.906 -13.23		1.00	0.00 0.00	3A7
ATOM	922 923	N O	VAL ARG	157 158	17.626 -14.6		1.00	0.00	3A7
ATOM ATOM	924	CA	ARG	158	18.365 -13.8		1.00	0.00	3A7
ATOM	925	СВ	ARG	158	19.590 -14.5		1.00	0.00	3A7
ATOM	926	CG	ARG	158	20.308 -13.8		1.00	0.00	3A7
ATOM	927	CD	ARG	158	21.475 -14.6		1.00	0.00	3A7 . 3A7
ATOM	928	NE	ARG	158	20.932 -15.9		1.00	0.00	. 3A7 3A7
ATOM	929 930	CZ NH1	ARG	158 158	21.742 -17.0 21.187 -18.2			0.00	3A7
ATOM ATOM	931		ARG	158	23.097 -16.9			0.00	3A7
ATOM	932	С	ARG	158	18.810 -12.5		1.00	0.00	3A7
MOTA	933	0	ARG	158	18.732 -11.4		1.00	0.00	3A7
MOTA	934	N	ASN	159	19.237 -12.5			0.00	3A7 3A7
ATOM	935	CA	ASN	159	19.621 -11.3 20.171 -11.6			0.00	3A7
ATOM ATOM	936 937	CB CG	ASN ASN	159 159	21.490 -12.4			0.00	3A7
ATOM	938		ASN	159	22.072 -12.6			0.00	3A7
ATOM	939		ASN	159	21.964 -12.9		1.00	0.00	3A7
ATOM	940	С	ASN	159	18.466 -10.4			0.00	3A7
ATOM	941	0	ASN.	159	18.606 -9.1			0.00	3A7 3A7
ATOM	942	N	LEU	160	17.267 -10.9			0.00	3A7
ATOM ATOM	943 944	CA CB	LEU	160 160	16.066 -10.1 14.972 -11.0			0.00	3A7
ATOM	945	CG	LEU	160	15.234 -11.4	57 36.902		0.00	3A7
ATOM	946		LEU	160	14.149 -12.4	30 36.402		0.00	3A7
ATOM	947	CD2	LEU	160	15.359 -10.2			0.00	3A7
ATOM	948	C	LEU	160	15.557 -9.6			0.00	3A7 3A7
ATOM	949	0	LEO	160	14.965 -8.5 15.836 -10.3			0.00	3A7
ATOM ATOM	950 951	N CA	ARG	161 161				0.00	3A7
ATOM	952	CB	ARG	161	15.773 -11.0			0.00	3A7
ATOM	953	CG	ARG	161	14.640 -12.0		1.00	0.00	3A7
MOTA	954	CD	ARG	161	14.752 -13.0				3A7
ATOM	955	NE	ARG	161	15.964 -13.9				3A7 3A7
MOTA	956	CZ	ARG	- 161	16.221 -15.0 17.333 -15.8				3A7
ATOM ATOM	957 958		ARG ARG	161 161	17.333 -13.8				3A7
MOTA	959	C	ARG	161	16.228 -8.7				3A7
ATOM	960	ō	ARG	161	15.673 -7.8	43 43.879	1.00		3A7
MOTA	961	N	ARG	162	17.510 -8.5				3A7
MOTA	962	CA	ARG	162	18.380 -7.4				3A7
MOTA	963	CB	ARG	162	19.851 -7.8 20.346 -8.9				3A7 3A7
MOTA	964	CG	ARG	162	20.346 -8.9	UU 13.02	, 1.00	0.00	JA,

ATOM	965	CD	ARG	162	21.838	-9.302	43.666	1.00	0.00	3A7
ATOM	966	NE	ARG	162	22.095	-9.696	42.242	1.00	0.00	3A7
ATOM	967	CZ	ARG	162	23.363	-9.855	41.755	1.00	0.00	3A7
MOTA	968	NH1	ARG	162	23.548	-10.141	40.433	1.00	0.00	3A7
MOTA	969	NH2	ARG	162	24.444	-9.724	42.577	1.00	0.00	3A7
ATOM	970	С	ARG	162	18.080	-6.236	42.355	1.00	0.00	3A7
ATOM	971	0	ARG	162	18.755	-5.220	42.500	1.00	0.00	3A7
ATOM	972	N	GLŲ	163	17.014	-6.247	41.519	1.00	0.00	3A7
ATOM	973	CA	GLU	163	16.615	-5.103	40.744	1.00	0.00	3A7
ATOM	974	CB	GLU	163	15.965	-5.504	39.413	1.00	0.00	3A7
ATOM	975	CG	GLU	163	16.981	-6.330	38.605	1.00	0.00	3A7
ATOM	976	CD	GLU	163	16.426	-6.716	37. <u>2</u> 46	1.00	0.00	3A7
ATOM	977	OE1	GLU	163	17.080	-6.372	36.227	1.00	0.00	3A7
ATOM	978	OE2	GLU	163	15.354	-7.376	37.210	1.00	0.00	3A7
ATOM	979	С	GLU	163	15.784	-4.183	41.582	1.00	0.00	3A7
ATOM	980	0	GLU	163	15.662	-2.998	41.288	1.00	0.00	3A7
MOTA	981	N	ALA	164	15.230	-4.708	42.699	1.00	0.00	3A7
ATOM	982	CA	ALA	164	14.728	-3.939	43.812	1.00	0.00	3A7
ATOM	983	CB	ALA	164	15.779	-2.963	44.394	1.00	0.00	. 3A7
ATOM	984	С	ALA	164	13.480	-3.200	43.529	1.00	0.00	3A7
ATOM	985	0	ALA	164	13.505	-1.993	43.644	1.00	0.00	3A7
ATOM	986	N	GLU	165	12.363	-3.878	43.176	1.00	0.00	3A7
MOTA	987	CA	GLU	165	10.993	-3.400	43.222	1.00	0.00	3A7
MOTA	988	СВ	GLU	165	10.561	-2.688	44.540	1.00	0.00	3A7
ATOM	989	CG	GLU	165	10.851	-3.510	45.809	1.00	0.00	3A7
MOTA	990	CD	GLU		10.308	-2.803	47.050	1.00	0.00	3A7
MOTA	991		GLU	165	9.757	-1.678	46.915	1.00	0.00	3A7 3A7
ATOM	992		GLU	165	10.441	-3.390	48.158	1.00	0.00	3A7
ATOM	993	С	GLU	165	10.541	-2.574	42.031		0.00	3A7 3A7
MOTA	994	0	GLU	165	9.403	-2.728	41.595 41.488	1.00	0.00	3A7
ATOM	995	N	THR	166	11.382	-1.661 -0.758	40.425	1.00	0.00	3A7
ATOM	996	CA	THR	166	10.979 10.351	0.509	40.423	1.00	0.00	3A7
ATOM	997	CB	THR	166	9.175	0.309	41.676	1.00	0.00	3A7
ATOM	998		THR	166	9.944	1.442	39.767	1.00	0.00	3A7
ATOM	999	CG2		166 166	12.235	-0.374	39.728	1.00	0.00	3A7
ATOM ATOM	1000 1001	С 0	THR	166	12.410	-0.652	38.547	1.00	0.00	3A7
	1001	И	GLY	167	13.141	0.230	40.560	1.00	0.00	3A7
ATOM ATOM	1002	CA	GLY	167	14.556	0.524	40.415	1.00	0.00	3A7
MOTA	1003	c	GLY	167	14.980	0.965	39.058	1.00	0.00	3A7
ATOM	1005	ŏ	GLY	167	15.037		38.750	1.00	0.00	3A7
ATOM	1006	N	LYS	168	15.246	-0.048	38.208	1.00	0.00	3A7
ATOM	1007	CA	LYS	168	15.423	0.121	36.801	1.00	0.00	3A7
ATOM	1008	СВ	LYS	168	16.887	-0.172	36.380	1.00	0.00	3A7
ATOM	1009	CG	LYS	168	17.309	0.475	35.050	1.00	0.00	3A7
ATOM	1010	CD	LYS	168	18.803	0.294	34.725	1.00	0.00	3A7
ATOM	1011	CE	LYS	168	19.236	-1.160	34.483	1.00	0.00	3A7
ATOM	1012	NZ	LYS	168	18.558	-1.731	33.297	1.00	0.00	3A7
ATOM	1013	C	LYS	168	14.438	-0.857	36.181	1.00	0.00	. 3A7
ATOM	1014	o	LYS	168	14.315	-1.969	36.694	1.00	0.00	3A7
MOTA	1015	N	PRO	169	13.751	-0.544	35.061	1.00	0.00	3A7
ATOM	1016	CA	PRO	169	13.228	-1.488	34.077	1.00	0.00	3A7
ATOM	1017	CD	PRO	169	13.706	0.834	34.565	1.00	0.00	3A7
ATOM	1018	CB	PRO	169	12.639	-0.568	33.005	1.00	0.00	3A7
MOTA	1019	CG	PRO	169	13.438	0.725	33.072	1.00	0.00	3A7
ATOM	1020	С	PRO	169	14.386	-2.289	33.508	1.00	0.00	3A7
MOTA	1021	0	PRO	169	15.533	-1.866	33.608	1.00	0.00	3A7
ATOM	1022	N	VAL	170	14.110	-3.480	32.963	1.00	0.00	3A7
ATOM	1023	CA	VAL	170	15.120	-4.462	32.688	1.00	0.00	3A7
MOTA	1024	CB	VAL	170	14.791	-5.773	33.379	1.00	0.00	3A7
MOTA	1025		VAL	170	15.992	-6.742	33.323	1.00	0.00	3A7
ATOM	1026		VAL	170	14.350	-5.485	34.825	1.00	0.00	3A7
MOTA	1027	C	VAL	170	15.190	-4.659	31.200	1.00	0.00	3A7
ATOM	1028	0	VAL	170	14.185	-4.556	30.501	1.00	0.00	3A7
MOTA	1029	N	THR	171	16.400	-4.984	30.690	1.00	0.00	3A7
MOTA	1030	CA	THR	171	16.616	-5.364	29.321	1.00	0.00	3A7
ATOM	1031	CB	THR	171	17.889	-4.784	28.730	1.00	0.00	3A7 3A7
MOTA	1032		THR	171	17.858	-3.368	28.857	1.00	0.00	3A7 3A7
ATOM	1033		THR	171	18.018	-5.145	27.233	1.00	0.00	3A7
ATOM	1034	C	THR	171	16.717	-6.854	29.319	1.00	0.00	3A7
ATOM	1035	0	THR	171	17.667	-7.434	29.839	1.00	0.00	3A7 3A7
ATOM	1036	N	LEU	172	15.716	-7.527	28.719	1.00	5.00	JA

ATOM	1037	CA	LEU	172	15.566 -8.	955 28.820	1.00	0.00	3A7
ATOM	1038	СВ	LEU	172		409 28.421	1.00	0.00	3A7
ATOM	1039	CG	LEU	172		735 29.139	1.00	0.00	3A7
MOTA	1040	CD1		172		664 30.670	1.00	0.00	3A7 3A7
ATOM	1041	CD2 C	LEU	172 172		378 28.501 705 27.991	1.00 1.00	0.00	3A7
ATOM ATOM	1042 1043	0	LEU	172	17.033 -10.		1.00	0.00	3A7
ATOM	1044	N	LYS	173		161 26.826	1.00	0.00	3A7
ATOM	1045	CA	LYS	173		803 25.952	1.00	0.00	3A7
ATOM	1046	CB	LYS	173		967 24.685	1.00	0.00	3A7
MOTA	1047	CG	LYS	173		687 23.605	1.00	0.00 0.00	3A7 3A7
ATOM	1048 1049	CĐ CE	LYS LYS	173 173		.825 22.357 .589 21.211	1.00	0.00	3A7
ATOM ATOM	1050	NZ	LYS	173		725 20.017	1.00	0.00	3A7
ATOM	1051	C.	LYS	173	19.296 -10.	057 26.620	1.00	0.00	3A7
ATOM	1052	0	LYS	173	19.912 -11.		1.00	0.00	3A7
ATOM	1053	N	HIS	174		103 27.472	1.00	0.00	3A7 3A7
ATOM	1054 1055	CA ND1	HIS	174 174		.190 28.204 .893 28.844	1.00	0.00	3A7
ATOM ATOM	1056	CG	HIS	174		783 29.521	1.00	0.00	3A7
ATOM	1057	СВ	HIS	174		846 28.865	1.00	0.00	3A7
ATOM	1058	NE2		174		664 30.996	1.00	0.00	3A7
ATOM	1059		HIS	174		645 30.834	1.00	0.00	3A7 3A7
ATOM	1060	CE1		174 174	24.824 -7. 20.970 -10.	.814 29.775 .255 29.275	1.00	0.00	3A7
ATOM ATOM	1061 1062	C O	HIS	174	21.877 -11.		1.00	0.00	3A7
ATOM	1063	N	VAL	175	19.954 -10.		1.00	0.00	3A7
ATOM	1064	CA	VAL	175	19.876 -11.		1.00	0.00	3A7
ATOM	1065	СВ	VAL	175	18.832 -10.		1.00	0.00	3A7 3A7
MOTA	1066		VAL	175	18.836 -11. 19.117 -9.	.586 33.568 .239 32.645	1.00	0.00	3A7
ATOM ATOM	1067 1068	C	VAL VAL	175 175	19.575 -12.		1.00	0.00	3A7
ATOM	1069	ŏ	VAL	175	20.055 -13.		1.00	0.00	3A7
ATOM	1070	N	PHE	176	18.769 -12.		1.00	0.00	3A7
ATOM	1071	CA	PHE	176	18.383 -14.		1.00	0.00	3A7
ATOM	1072	CB	PHE	176	17.044 -13. 15.984 -14.		1.00	0.00	3A7 3A7
ATOM ATOM	1073 1074	CG CD1	PHE	176 176	15.271 -12		1.00	0.00	3A7
ATOM	1075		PHE	176	15.760 -15.		1.00	0.00	3A7
ATOM	1076	CE1	PHE	176	14.380 -12		1.00	0.00	3A7
ATOM	1077		PHE	176	14.857 -15.		1.00	0.00	3A7
ATOM	1078	CZ	PHE	176 - 176	14.171 -14. 19.411 -14.		1.00	0.00	3A7 3A7
ATOM ATOM	1079 1080	С 0	PHE	176	19.429 -15.			0.00	3A7
ATOM	1081	N	GLY	177	20.328 -13.			0.00	3A7
MOTA	1082	CA	GLY	177	21.447 -14		1.00	0.00	3A7
ATOM	1083	C.	GLY	177	22.530 -14.			0.00	3A7 3A7
ATOM ATOM	1084 1085	O N	GLY ALA	177 178	23.231 -15. 22.657 -14.			0.00	3A7
ATOM	1086	CA	ALA	178	23.616 -14			0.00	3A7
ATOM	1087	СВ	ALA	178	23.639 -13	.426 31.327		0.00	3A7
ATOM	1088	С	ALA	178	23.303 -15			0.00	3A7
ATOM	1089	0	ALA	178	24.178 -16.			0.00	3A7
ATOM ATOM	1090 1091	N CA	TYR TYR	179 179	22.004 -16. 21.522 -17.			0.00	3A7 3A7
ATOM	1092	СВ	TYR	179	19.979 -17			0.00	3A7
ATOM	1093	CG	TYR	179	19.104 -18	.432 31.952		0.00	3A7
ATOM	1094		TYR	179	18.538 -18			0.00	3A7
ATOM	1095 1096		TYR TYR	179	18.795 -19 17.873 -20			0.00	3A7 3A7
MOTA MOTA	1095		TYR	179 179	18.128 -20			0.00	3A7
ATOM	1098	CZ	TYR	179	17.709 -20			0.00	3A7
MOTA	1099	ОН	TYR	179	17.108 -22			0.00	3A7
ATOM	1100	C	TYR	179	21.881 -18			0.00	3A7 3A7
ATOM	1101 1102	O N	TYR SER	179 180	22.420 -19 21.607 -18			0.00	3A7
ATOM ATOM	1102	CA	SER	180	21.758 -19			0.00	3A7
ATOM	1104	СВ	SER	180	20.943 -19		1.00	0.00	3A7
ATOM	1105	OG	SER	180	21.331 -18			0.00	3A7
MOTA	1106	C	SER	180	23.198 -19			0.00	3A7 3A7
MOTA MOTA	1107 1108	O N	SER	180 181	23.565 -21 24.084 -18	.010 28.278 .834 28.319		0.00	3A7

ATOM	1109	CA	MET	181	25.507	-19.052	28.132	1.00	0.00	3A7
ATOM	1110	СВ	MET	181	26.246		27.978	1.00	0.00	3A7
MOTA	1111	CG	MET	181	25.986		26.568	1.00	0.00	3A7 3A7
ATOM	1112	SD	MET	181	26.894 25.919		26.130 27.203	1.00	0.00	3A7
MOTA MOTA	1113 1114	CE C	Met Met	181 181	26.127		29.282	1.00	0.00	3A7
ATOM	1115	o	MET	181	26.923		29.117	1.00	0.00	3A7
ATOM	1116	N	ASP	182	25.695		30.493	1.00	0.00	3A7
MOTA	1117	CA	ASP	182	26.174		31.695	1.00	0.00	3A7
MOTA	1118	СВ	ASP	182	25.809		32.908	1.00	0.00	3A7 3A7
ATOM	1119	CG	ASP ASP	182 182	26.545 27.380		32.877 31.961	1.00	0.00	3A7
MOTA MOTA	1120 1121		ASP	182	26.276		33.788	1.00	0.00	3A7
ATOM	1122	c	ASP	182	25.645		31.886	1.00	0.00	3A7
MOTA	1123	0	ASP	182		-22.258	32.382	1.00	0.00	3A7
ATOM	1124	N	VAL	183	24.401		31.448	1.00	0.00	3A7 3A7
ATOM	1125	CA	VAL	183 183		-23.084 -23.173	31.514 31.124	1.00	0.00	3A7
ATOM ATOM	1126 1127	CB CG1	VAL VAL	183		-24.632	30.984	1.00	0.00	3A7
ATOM	1128		VAL	183		-22.468	32.200	1.00	0.00	3A7
ATOM	1129	С	VAL	183		-24.016	30.610	1.00	0.00	3A7
MOTA	1130	0	VAL	183		-25.103	31.027	1.00	0.00	3A7 3A7
ATOM	1131	N	ILE	184		-23.597 -24.395	29.353 28.439	1.00	0.00 0.00	3A7
ATOM ATOM	1132 1133	CA CB	ILE	184 184		-23.816	27.039	1.00	0.00	3A7
ATOM	1134		ILE	184		-24.750	26.093	1.00	0.00	3A7
ATOM	1135		ILE	184		-23.617	26.489	1.00	0.00	3A7
MOTA	1136	CD	ILE	184		-24.898	26.404	1.00	0.00	3A7 3A7
ATOM	1137	C	ILE	184		-24.561 -25.652	28.928 28.859	1.00	0.00	3A7
ATOM ATOM	1138 1139	O N	ILE	184 185		-23.489	29.486	1.00	0.00	3A7
ATOM	1140	CA	THR	185		-23.511	30.002	1.00	0.00	3A7
ATOM	1141	СВ	THR	185		-22.111	30.359	1.00	0.00	3A7
MOTA	1142		THR	185		-21.307	29.187	1.00	0.00	3A7 3A7
ATOM	1143		THR	185		-22.108 -24.418	30.943 31.192	1.00	0.00	3A7
ATOM ATOM	1144 1145	С О	THR	185 185		-25.166	31.343	1.00	0.00	3A7
ATOM	1146	N	SER	186		-24.404	32.066	1.00	0.00	3A7
ATOM	1147	CA	SER	186		-25.188	33.262	1.00	0.00	3A7
ATOM	1148	CB	SER	186		-24.719	34.259	1.00	0.00 0.00	3A7 3A7
ATOM	1149	oG C	SER	186 186		-23.412 -26.655	34.719 33.000	1.00	0.00	3A7
ATOM ATOM	1150 1151	ò	SER SER	186		-27.500	33.598	1.00	0.00	3A7
ATOM	1152	N	THR	187		-27.006	32.060	1.00	0.00	3A7
MOTA		CA	THR	187		-28.386	31.711	1.00	0.00	3A7
ATOM	1154	CB	THR			-28.580	30.943	1.00	0.00	3A7 3A7
ATOM ATOM	1155 1156		THR	187 187		-27.748 -28.285	29.789 31.861	1.00	0.00	3A7
ATOM	1157	C	THR	187		-28.983	30.897	1,00	0.00	3A7
MOTA	1158	0	THR	187		-30.195	30.899	1.00	0.00	3A7
MOTA	1159	N	SER	188		-28.115	30.176	1.00	0.00	3A7
ATOM	1160	CA	SER	188		-28.556 -27.697	29.280 27.991	1.00	0.00	3A7 3A7
ATOM ATOM	1161 1162	CB OG	SER	188 188		-26.347	28.250		0.00	3A7
ATOM	1163	c	SER	188		-28.690	29.970	1.00	0.00	3A7
ATOM	1164	0	SER	188		-29.681	29.768	1.00	0.00	3A7
MOTA	1165	N	PHE	189		-27.672	30.766	1.00	0.00	3A7 3A7
ATOM ATOM	1166 1167	CA CB	PHE	189 189		-27.581 -26.363	31.256 30.732	1.00	0.00	3A7
ATOM	1168	CG	PHE	189		-26.027	29.300	1.00	0.00	3A7
ATOM	1169		PHE	189		-24.694	28.976	1.00	0.00	3A7
ATOM	1170	CD2	PHE	189		-26.986	28.292	1.00	0.00	3A7
ATOM	1171		PHE	189		-24.317	27.665	1.00	0.00	3A7 3A7
ATOM ATOM	1172 1173	CE2	PHE	189 189		-26.618 -25.284	26.984 26.668	1.00	0.00	3A7
ATOM	1174	C	PHE	189		-27.463	32.762	1.00	0.00	3A7
ATOM	1175	ŏ	PHE	189	33.993	-27.441	33.361	1.00	0.00	3A7
ATOM	1176	N	GLY	190		-27.378	33.435	1.00	0.00	3A7
ATOM	1177	CA	GLY	190		-27.345 -25.956	34.883 35.418	1.00	0.00	3A7 3A7
ATOM ATOM	1178 1179	0	<b>GLY</b>	190 190		-25.956	35.280	1.00		3A7
ATOM	1180	N	VAL			-25.744	36.044			3A7

ATOM	1181	CA	VAL	191	33.597	-24.510	36.596	1.00	0.00	3A7
ATOM	1182	CB	VAL	191	33.426	-23.250	35.727	1.00	0.00	3A7
ATOM	1183	CG1		191		-22.372	36.078	1.00	0.00	3A7
MOTA	1184	CG2		191		-22.424	35.812	1.00	0.00	3A7 3A7
ATOM	1185	C	VAL	191 191		-24.310 -24.551	38.012 38.325	1.00	0.00	3A7
ATOM ATOM	1186 1187	O N	VAL SER	192		-23.844	38.900	1.00	0.00	3A7
ATOM	1188	CA	SER	192		-23.531	40.281	1.00	0.00	3A7
ATOM	1189	CB	SER	192	34.779	-24.116	41.252	1.00	0.00	3A7
ATOM	1190	OG	SER	192		-25.534	41.156	1.00	0.00	3A7 3A7
ATOM	1191	C	SER	192		-22.032 -21.317	40.410 39.501	1.00	0.00	3A7
ATOM ATOM	1192 1193	N O	SER	192 193		-21.524	41.572	1.00	0.00	3A7
ATOM	1194	CA	ILE	193		-20.109	41.867	1.00	0.00	3A7
ATOM	1195		ILE	193		-19.756	42.671	1.00	0.00	3A7
MOTA	1196		ILE	193		-18.225	42.861	1.00	0.00	3A7
MOTA	1197		ILE	193		-20.322 -19.784	41.992 40.581	1.00	0.00	3A7 3A7
ATOM ATOM	1198 1199	CD C	ILE	193 193		-19.720	42.618	1.00	0.00	3A7
ATOM	1200	ŏ	ILE	193		-19.967	43.816	1.00	0.00	3A7
ATOM	1201	N	ASP	194	35.344	-19.102	41.887	1.00	0.00	3A7
ATOM	1202	CA	ASP	194		-18.685	42.420	1.00	0.00	3A7
ATOM	1203	CB	ASP	194		-19.786	42.267	1.00	0.00 0.00	3A7 3A7
MOTA	1204	CG OD1	ASP	194 194		-19.433 -19.270	43.034 44.280	1.00	0.00	3A7
ATOM ATOM	1205 1206		ASP	194		-19.326	42.381	1.00	0.00	3A7
ATOM	1207	c	ASP	194		-17.442	41.654	1.00	0.00	3A7
MOTA	1208	0	ASP	194		-16.608	42.141	1.00	0.00	3A7
MOTA	1209	N	SER	195		-17.299	40.420	1.00	0.00	3A7 3A7
ATOM	1210	CA	SER	195 195		-16.163 -16.561	39.548 38.055	1.00	0.00	3A7
ATOM ATOM	1211 1212	CB OG	SER	195		-17.464	37.811	1.00	0.00	3A7
ATOM	1213	c	SER	195		-15.185	39.763	1.00	0.00	3A7
MOTA	1214	0	SER	195		-15.547	40.256	1.00	0.00	3A7
MOTA	1215	N	LEU	196		-13.902	39.386	1.00	0.00	3A7 3A7
ATOM	1216 1217	CA CB	LEU	196 196		-12.813 -11.523	39.580 40.138	1.00	0.00	3A7
ATOM ATOM	1217	·CG	LEU	196		-11.639	41.551	1.00	0.00	3A7
ATOM	1219		LEU	196		-12.190	42.599	1.00	0.00	3A7
ATOM	1220	CD2	LEU	196		-12.399	41.574	1.00	0.00	3A7
MOTA	1221	С	LEU	196		-12.481	38.258	1.00	0.00	3A7 3A7
ATOM	1222 1223	O N	LEU ASN	196 197		-11.334 -13.503	38.022 37.366	1.00	0.00	3A7
ATOM ATOM	1223	CA	ASN	197		-13.455	36.068	1.00	0.00	3A7
ATOM	1225	СВ	ASN	197		-12.846	36.138	1.00	0.00	3A7
ATOM	1226	CG	ASN	197		-13.111	34.865	1.00	0.00	3A7
ATOM	1227		ASN	197		-14.206	34.295	1.00	0.00	3A7 3A7
ATOM	1228 1229	ND2	ASN ASN	197 197		-12.069 -12.714	34.431 35.072	1.00	0.00	3A7
ATOM ATOM	1230	0	ASN	197		-11.770	34.419	1.00	0.00	3A7
ATOM	1231	N	ASN	198	35.541	-13.134	34.960	1.00	0.00	3A7
MOTA	1232	ÇA	ASN	198		-12.476	34.117	1.00	0.00	3A7
ATOM	1233	CB	ASN	198	37.878	-12.191	34.815	1.00	0.00	3A7 3A7
ATOM ATOM	1234 1235	CG OD1	ASN ASN	198 198		-11.423 -11.949	36.121 37.214	1.00	0.00	3A7
ATOM	1236		ASN	198		-10.153	35.986	1.00	0.00	3A7
ATOM	1237	С	ASN	198		-13.246	32.825	1.00	0.00	3A7
MOTA	1238	0	ASN	198		-12.598	31.789	1.00	0.00	3A7
MOTA	1239	N	PRO	199		-14.562	32.735	1.00	0.00	3A7 3A7
MOTA MOTA	1240 1241	CA CD	PRO PRO	199 199		-15.242 -15.415	31.473 33.865	1.00	0.00	3A7
ATOM	1241	CB	PRO	199		-16.553	31.866	1.00	0.00	3A7
MOTA	1243	CG	PRO	199	38.421	-16.338	33.313	1.00	0.00	3A7
ATOM	1244	С	PRO	199		-15.538	30.731	1.00	0.00	3A7
ATOM	1245	0	PRO	199		-15.766	29.524	1.00	0.00	3A7 3A7
ATOM ATOM	1246 1247	N CA	GLN GLN	200 200		-15.560 -15.967	31.441 30.914	1.00	0.00	3A7
MOTA	1247	CB	GLN	200		-16.559	32.023	1.00	0.00	3A7
MOTA	1249	CG	GLN	200		-17.173	31.515	1.00	0.00	3A7
MOTA	1250	CD	GLN	200		-17.885	32.668	1.00	0.00	3A7
MOTA	1251		GLN	200		-19.110	32.645	1.00	0.00	3A7 3A7
MOTA	1252	NE2	GLN	200	0.150 کا	-17.085	33.690	1.00	0.00	3A /

ATOM	1253	С	GLN	200	32.815	-14.819	30.232	1.00	0.00	3A7
	1254	ŏ	GLN	200		-15.035	29.233	1.00	0.00	3A7
ATOM				201		-13.568	30.743	1.00	0.00	3A7
MOTA	1255	N	ASP				30.219	1.00	0.00	3A7
ATOM	1256	CA	ASP	201		-12.384	-			3A7
ATOM	1257	СВ	ASP	201		-11.254	31.288	1.00	0.00	
ATOM	1258	CG	ASP	201	31.197	-10.174	30.927	1.00	0.00	3A7
ATOM	1259	ODI	ASP	201	31.610	-8.994	30.772	1.00	0.00	3A7
ATOM	1260		ASP	201	29.992	-10.520	30.805	1.00	0.00	3A7
		c	ASP	201		-11.859	28.899	1.00	0.00	3A7
ATOM	1261						28.095	1.00	0.00	3A7
MOTA	1262	0	ASP	201		-11.342			0.00	3A7
ATOM	1263	N	PRO	202		-11.966	28.590	1.00		
ATOM	1264	CA	PRO	202	34.768	-11.731	27.282	1.00	0.00	3A7
ATOM	1265	CD	PRO	202	35.191	-11.898	29.612	1.00	0.00	3A7
MOTA	1266	СВ	PRO	202	36.280	-11.790	27.543	1.00	0.00	3A7
ATOM	1267	CG	PRO	202		-11.259	28.958	1.00	0.00	3A7
		Č	PRO	202		-12.755	26.270	1.00	0.00	3A7
MOTA	1268					-12.386	25.126	1.00	0.00	3A7
MOTA	1269	0	PRO	202						3A7
ATOM	1270	N	PHE	203		-14.041	26.662	1.00	0.00	
MOTA	1271	CA	PHE	203	33.692	-15.113	25.807	1.00	0.00	3A7
ATOM	1272	CB	PHE	203	33.533	-16.402	26.628	1.00	0.00	3A7
ATOM	1273	CG	PHE	203	33.530	-17.655	25.800	1.00	0.00	3A7
ATOM	1274		PHE	203	34.701	-18.401	25.685	1.00	0.00	3A7
			PHE	203		-18.126	25.192	1.00	0.00	3A7
MOTA	1275					-19.599	24.981	1.00	0.00	3A7
MOTA	1276		PHE	203						3A7
ATOM	1277			203		-19.316	24.471	1.00	0.00	
ATOM	1278	ÇZ	PHE	203	33.547	-20.060	24.377	1.00	0.00	3A7
MOTA	1279	С	PHE	203	32.360	-14.780	25.173	1.00	0.00	3A7
ATOM	1280	0	PHE	203	32.125	-15.040	23.999	1.00	0.00	3A7
ATOM	1281	N	VAL	204		-14.147	25.959	1.00	0.00	3A7
	1282	CA	VAL	204		-13.686	25.564	1.00	0.00	3A7
MOTA						-12.914	26.710	1.00	0.00	3A7
ATOM	1283	CB	VAL	204						3A7
ATOM	1284		VAL	204		-12.240	26.286	1.00	0.00	
ATOM	1285	CG2	VAL	204		-13.845	27.927	1.00	0.00	3A7
ATOM	1286	С	VAL	204	30.210	-12.702	24.430	1.00	0.00	3A7
ATOM	1287	0	VAL	204	29.521	-12.835	23.424	1.00	0.00	3A7
ATOM	1288	N	GLU	205	31.077	-11.674	24.576	1.00	0.00	3A7
ATOM	1289	CA	GLU	205		-10.607	23.617	1.00	0.00	3A7
				205	32.215		24.146	1.00	0.00	3A7
ATOM	1290	CB	GLU					1.00	0.00	3A7
ATOM	1291	CG	GLU	205	32.242		23.327			
ATOM	1292	CD	GLU	205	33.217		23.979	1.00	0.00	3A7
ATOM	1293	OE1	GLU	205	32.974		25.153	1.00	0.00	3A7
ATOM	1294	OE2	GLU	205	34.219	-6.896	23.310	1.00	0.00	3A7
ATOM	1295	С	GLU	205	31.739	-11.106	22.289	1.00	0.00	3A7
ATOM	1296	0	GLU	205	31.308	-10.646	21.238	1.00	0.00	3A7
ATOM	1297	N	ASN	206		-12.123	22.316	1.00	0.00	3A7
		CA		206		-12.741	21.134	1.00	0.00	3A7
ATOM	1298		ASN						0.00	3A7
ATOM	1299	СВ	ASN	206		-13.657	21.467	1.00		
ATOM	1300	CG	ASN	206		-12.819	22.025	1.00	0.00	3A7
ATOM	1301	QD1	ASN	206		-12.848	23.224	1.00	0.00	. 3A7
ATOM	1302	ND2	ASN	206	36.155	-12.023	21.120	1.00	0.00	3A7
ATOM	1303	С	ASN	206	32.151	-13.539	20.380	1.00	0.00	3A7
ATOM	1304	0	ASN	206		-13.337	19.182	1.00	0.00	3A7
ATOM	1305	N	THR	207		-14.452	21.067	1.00	0.00	3A7
	1306	CA	THR	207		-15.301	20.464	1.00	0.00	3A7
ATOM						-16.188	21.502	1.00	0.00	3A7
ATOM	1307	CB	THR	207						3A7
MOTA	1308		THR	207		-16.917	22.199	1.00	0.00	
ATOM	1309		THR	207		-17.201	20.851	1.00	0.00	3A7
ATOM	1310	С	THR	207	29.346	-14.492	19.768	1.00	0.00	3A7
ATOM	1311	0	THR	207	28.951	-14.790	18.646	1.00	0.00	3A7
ATOM	1312	N	LYS	208	28.929	-13.379	20.411	1.00	0.00	3A7
ATOM	1313	CA	LYS	208		-12.459	19.890	1.00	0.00	3A7
			LYS	208		-11.413	20.954	1.00	0.00	3A7
ATOM	1314	CB				-11.413		1.00	0.00	3A7
ATOM	1315	CG	LYS	208			20.601			
ATOM	1316	CD	LYS	208	25.914		21.741	1.00	0.00	3A7
ATOM	1317	CE	LYS	208	26.80		22.018	1.00	0.00	3A7
ATOM	1318	NZ	LYS	208	28.077	7 -8.751	22.673	1.00	0.00	3A7
ATOM	1319	С	LYS	208	28.389	-11.760	18.619	1.00	0.00	3A7
ATOM	1320	ō	LYS	208		5 -11.653	17.675	1.00	0.00	3A7
ATOM	1321	N	LYS	209		-11.316	18.536	1.00	0.00	3A7
			LYS	209		-10.686	17.348	1.00	0.00	3A7
ATOM	1322	CA							0.00	3A7
MOTA	1323	СВ	LYS	209		2 -10.129	17.587	1.00		
MOTA	1324	CG	LYS	209	31.660	8.877	18.478	1.00	0.00	3A7

АТОМ	1325	CD	LYS	209	33.007	-8.133	18.418	1.00	0.00	3A	7
ATOM	1326	CE	LYS	209	34.227	-8.963	18.843	1.00	0.00	3A	
ATOM	1327	NZ	LYS	209	34.144	-9.343	20.270	1.00	0.00	3A	
MOTA	1328	С	LYS	209	30.275		16.153	1.00	0.00	3A 3A	
ATOM	1329	0	LYS	209	29.942 30.662		15.031 16.376	1.00	0.00	3A	
MOTA	1330 1331	N CA	LEU	210 210	30.592		15.391	1.00	0.00	3A	
ATOM ATOM	1332	CB	LEU	210	30.985		16.011	1.00	0.00	3A	7
ATOM	1333	CG	LEU	210	31.127		15.108	1.00	0.00	3A	
ATOM	1334		LEU	210	31.072		16.013	1.00	0.00	3A	
ATOM	1335	CD2	LEU	210	30.134		13.954	1.00	0.00	3A	
MOTA	1336	Ç	LEU	210	29.217		14.809	1.00	0.00	3A 3A	
ATOM	1337	0	LEU	210 211	29.056 28.185		13.595 15.680	1.00	0.00	3A	
ATOM ATOM	1338 1339	N CA	LEU	211	26.814		15.302	1.00	0.00	3A	
ATOM	1340	СВ	LEU	211	25.835		16.480	1.00	0.00	3A	.7
ATOM	1341	CG	LEU	211	26.035	-15.159	17.726	1.00	0.00	3A	
MOTA	1342	CD1	LEU	211	24.820		18.669	1.00	0.00	3A	
ATOM	1343		LEU	211	26.398		17.396	1.00	0.00	3A 3A	
ATOM	1344	C	LEU	211	26.271 25.479		14.274 13.418	1.00	0.00	3A	
ATOM ATOM	1345 1346	O N	LEU ARG	211 212	26.667		14.324	1.00	0.00	3A	
MOTA	1347	CA	ARG	212	26.196		13.386	1.00	0.00	ЗА	7
ATOM	1348	СВ	ARG	212	25.985	-9.737	14.028	1.00	0.00	3A	
ATOM	1349	CG	ARG	212	27.103	-9.170	14.927	1.00	0.00	3A	
ATOM	1350	CD	ARG	212	28.270	-8.508	14.183	1.00	0.00	3A 3A	
ATOM	1351	NE	ARG	212	29.078 30.393	-7.724 -7.406	15.175 14.970	1.00	0.00	3A	
ATOM ATOM	1352 1353	CZ NH1	ARG	212 212	31.075	-7.901	13.898	1.00	0.00	37	
ATOM	1354		ARG	212	31.031	-6.581	15.851	1.00	0.00	3A	١7
ATOM	1355	С	ARG	212	27.097	-11.091	12.169	1.00	0.00	34	
ATOM	1356	0	ARG	212		-11.083	12.272	1.00	0.00	34	
MOTA	1357	N	PHE	213		-11.117	10.976	1.00	0.00	3A 3A	
MOTA	1358	CA CB	PHE	213 213	27.428	-11.263 -9.944	9.611 8.921	1.00	0.00	32	
ATOM ATOM	1359 1360	CG	PHE	213	28.597	-9.221	9.541	1.00	0.00	32	
ATOM	1361		PHE	213	28.391	-8.264	10.535	1.00	0.00	32	
MOTA	1362	CD2	PHE	213	29.890	-9.399	9.039	1.00	0.00		
ATOM	1363		PHE	213	29.455	-7.517	11.032	1.00	0.00	· 31	
ATOM	1364		PHE	213	30.959 30.741	-8.666 -7.723	9.546 10.544	1.00	0.00	37	
ATOM ATOM	1365 1366	CZ C	PHE	213 213		-12.408	9.426	1.00	0.00	37	
ATOM	1367	ŏ	PHE	213		-12.215	9.209	1.00	0.00	37	47
ATOM	1368	N	ASN	214	27.395	-13.649	9.491	1.00	0.00	37	
. ATOM	1369	CA	ASN	214		-14.839	9.165	1.00	0.00		47 47
ATOM	1370	CB	ASN	214		-15.372	10.314 9.818	1.00	0.00		47 47
ATOM	1371 1372	CG	ASN ASN	214 214		-16.484 -16.242	8.972	1.00	0.00		A7
ATOM ATOM	1373		ASN	214		-17.720	10.370	1.00	0.00		A7
ATOM	1374	C	ASN	214		-15.863	8.671	1.00	0.00		A7
MOTA	1375	0	ASN	214		-16.351	7.565	1.00	0.00		A7
MOTA	1376	N	PRO	215		-16.260	9.344	1.00	0.00		A7 A7
MOTA	1377	CA	PRO	215 215		-17.305 -15.929	8.858 10.728	1.00	0.00	_	A7
ATOM ATOM	1378 1379	CD CB	PRO PRO	215		-17.865	10.125	1.00	0.00		A7
ATOM	1380	CG	PRO	215		-17.241	11.310	1.00	0.00	37	A7
ATOM	1381	С	PRO	215		-16.681	7.893	1.00	0.00		A7
ATOM	1382	Ο,	PRO	215		-15.982	8.353	1.00	0.00		A7
ATOM	1383	N	LEU	216		-16.921	6.560	1.00	0.00		A7 A7
ATOM	1384 1385	CA CB	LEU	216 216		-16.424 -16.737	5.463 5.575	1.00	0.00		A7
ATOM ATOM	1385	CG	LEU	216		-18.224	5.393	1.00	0.00		A7
ATOM	1387		LEU	216		-18.782	4.017	1.00	0.00	3	<b>A</b> 7
ATOM	1388		LEU	216		-19.148	6.540	1.00	0.00		A7
ATOM	1389	С	LEU	216		-14.925	5.304	1.00	0.00		A7 A7
ATOM	1390	0	LEU	216		-14.143 -14.501	5.980 4.392	1.00	0.00		A7
ATOM ATOM	1391 1392	N CA	ASP ASP	217 217		-14.501	4.192	1.00	0.00		A7
ATOM	1392	CB	ASP	217		-12.608	5.013	1.00	0.00		A7
ATOM	1394	CG	ASP	217		-13.427	4.786	1.00	0.00		A7
ATOM	1395		ASP	217		-12.833	4.285	1.00	0.00		A7
ATOM	1396	OD2	ASP	217	27.390	-14.641	5.118	1.00	0.00		A7

ATOM	1397	С	ASP	217	25.056	-12.846	2.709	1.00	0.00	3A7
ATOM	1398	ō	ASP	217	26.126		2.166	1.00	0.00	3A7
ATOM	1399	N	PRO	218	24.053	-12.282	2.013	1.00	0.00	3A7
ATOM	1400	CA	PRO	218	24.193		0.691	1.00	0.00	3A7
MOTA	1401	CD	PRO	218	22.655		2.382	1.00	0.00	3A7 3A7
MOTA	1402	CB	PRO	218	22.746		0.203 1.050	1.00	0.00	3A7
ATOM	1403	CG	PRO	218	21.908 · 24.945 ·		0.782	1.00	0.00	3A7
ATOM	1404 1405	C O	PRO PRO	218 218	24.911	-9.730	1.833	1.00	0.00	3A7
ATOM ATOM	1406	N	PHE	219	25.621	-9.950	-0.316	1.00	0.00	3A7
ATOM	1407	CA	PHE	219	26.432	-8.745	-0.344	1.00	0.00	3 <b>A</b> 7
ATOM	1408	CB	PHE	219	27.591	-8.800	-1.373	1.00	0.00	3A7
ATOM	1409	CG	PHE	219	28.495	-9.952	-1.047	1.00	0.00	3A7
ATOM	1410	CD1	PHE	219	29.296	-9.917	0.094	1.00	0.00	3A7
MOTA	1411	CD2		219	28.551		-1.881	1.00	0.00	3A7 3A7
ATOM	1412	CEI		219	30.140 29.393		0.400 -1.578	1.00 1.00	0.00 0.00	3A7
MOTA	1413	CE2 CZ	PHE	219 219	30.189		-0.437	1.00	0.00	3A7
ATOM ATOM	1414 1415	C	PHE	219	25.587	-7.501	-0.570	1.00	0.00	3A7
ATOM	1416	ŏ	PHE	219	25.626	-6.607	0.273	1.00	0.00	3A7
ATOM	1417	N	VAL	220	24.790	-7.366	-1.669	1.00	0.00	3A7
ATOM	1418	CA	VAL	220	24.617	-8.245	-2.807	1.00	0.00	3A7
ATOM	1419	СВ	VAL	220	23.148	-8.591	-3.051	1.00	0.00	3A7
MOTA	1420	CG1		220	22.271	-7.323	-3.127	1.00	0.00	3A7
ATOM	1421	CG2		220	22.991	-9.517	-4.277 -3.983	1.00	0.00	. 3A7 3A7
ATOM	1422	C	VAL	220	25.287 25.799	-7.570 -8.235	-4.883	1.00	0.00	3A7
ATOM ATOM	1423 1424	O N	VAL LEU	220 221	25.336	-6.211	-3.963	1.00	0.00	3A7
ATOM	1425	CA	LEU	221	26.163	-5.403	-4.835	1.00	0.00	3A7
ATOM	1426	СВ	LEU	221	25.390	-4.284	-5.597	1.00	0.00	3A7
ATOM	1427	CG	LEU	221	24.479	-4.750	-6.764	1.00	0.00	3A7
ATOM	1428	CD1		221	25.258	-5.539	-7.835	1.00	0.00	3A7
ATOM	1429		LEU	221	23.213	-5.501	-6.317	1.00	0.00	3A7
ATOM	1430	C	LEU	221	27.196	-4.792	-3.913	1.00	0.00	3A7 3A7
ATOM	1431	0	LEU	221 222	27.565 27.682	-5.391 -3.567	-2.904 -4.239	1.00	0.00	3A7
ATOM ATOM	1432 1433	N CA	SER SER	222	28.622	-2.816	-3.435	1.00	0.00	3A7
ATOM	1434	CB	SER	222	29.722	-2.139	-4.284	1.00	0.00	3A7
ATOM	1435	OG	SER	222	30.472	-3.121	-4.985	1.00	0.00	3A7
ATOM	1436	С	SER	222	27.841	-1.762	-2.698	1.00	0.00	3A7
ATOM	1437	0	SER	222	27.764	-0.612	-3.127	1.00	0.00	3A7
ATOM	1438	N	ILE	223	27.222	-2.164	-1.561	1.00	0.00	3A7
ATOM	1439	CA	ILE	223	26.322	-1.338 -2.017	-0.788 -0.555	1.00	0.00	3A7 3A7
MOTA	1440 1441	CB	ILE	223 223	24.971 25.156	-3.487	-0.110	1.00	0.00	3A7
ATOM ATOM	1442		ILE	223	24.042	-1.193	0.374	1.00	0.00	3A7
ATOM	1443	CD	ILE	223	22.603	-1.718	0.416	1.00	0.00	3 <b>A</b> 7
ATOM	1444	С	ILE	223	27.019	-0.926	0.488	1.00	0.00	3A7
ATOM	1445	0	ILE	223 .	27.093	0.266	0.787	1.00	0.00	3A7
ATOM	1446	N	LYS	224	27.556	-1.893	1.271	1.00	0.00	3A7
MOTA	1447	CA	LYS	224	28.263	-1.581	2.490	1.00	0.00	. 3A7 3A7
ATOM	1448 1449	CB CG	LYS LYS	224 224	27.339 28.088	-1.185 -0.528	3.674 4.849	1.00	0.00	3A7
ATOM ATOM	1450	CD	LYS	224	27.190	-0.187	6.049		0.00	3A7
ATOM	1451	CE	LYS	224	26.740	-1.411	6.861	1.00	0.00	3 <b>A</b> 7
ATOM	1452	NZ	LYS	224	27.901	-2.112	7.458	1.00	0.00	3A7
MOTA	1453	C	LYS	224	29.052	-2.796	2.890	1.00	0.00	3A7
MOTA	1454	0	LYS	224	30.070	-2.683	3.572	1.00	0.00	3A7
MOTA	1455	N	VAL	225	28.582	-4.008	2.483	1.00	0.00	3A7 3A7
ATOM	1456	CA	VAL	225	29.124	-5.288	2.907 2.746	1.00	0.00	3A7
ATOM ATOM	1457 1458	CB	VAL VAL	225 225	28.125 28.683	-6.430 -7.731	3.365	1.00	0.00	3A7
ATOM	1459		VAL	225	26.805	-6.017	3.429	1.00	0.00	3A7
ATOM	1460	C	VAL	225	30.398	-5.583	2.147	1.00	0.00	3A7
ATOM	1461	ō	VAL	225	31.486	-5.449	2.708	1.00	0.00	3A7
MOTA	1462	N	PHE	226	30.271	-5.986	0.851	1.00	0.00	3A7
ATOM	1463	CA	PHE	226	31.349	-6.182	-0.106	1.00	0.00	3A7
MOTA	1464	CB	PHE	226	32.367	-4.997	-0.098	1.00	0.00	3A7 3A7
ATOM	1465	CG	PHE	226 226	33.203 34.585	-4.921 -5.107	-1.346 -1.283	1.00	0.00	3A7
ATOM ATOM	1466 1467		PHE	226	32.615	-4.631	-2.578	1.00	0.00	3A7
ATOM	1468		PHE		35.365	-5.025	-2.432	1.00	0.00	3A7

ATOM	1469	CE2	PHE	226	33.393	-4.550	-3.730	1.00	0.00	3A7
ATOM	1470	CZ	PHE	226	34.768	-4.749	-3.658	1.00	0.00	3A7
ATOM	1471	С	PHE	226	32.059	-7.514	0.144	1.00	0.00	3A7 3A7
ATOM	1472	0	PHE	226	32.151	-7.943 -8.198	1.295 -0.871	1.00	0.00	3A7 3A7
ATOM	1473 1474	N CA	PRO PRO	227 227	32.610 33.431	-9.392	-0.698	1.00	0.00	3A7
ATOM ATOM	1475	CD	PRO	227	32.111	-8.089	-2.237	1.00	0.00	3A7
ATOM	1476	СB	PRO	227	33.602	-9.944	-2.123	1.00	0.00	3A7
ATOM	1477	CG	PRO	227	32.349	-9.465	-2.857	1.00	0.00	3A7
ATOM	1478	С	PRO	227	34.778	-9.081	-0.061	1.00	0.00	3A7 3A7
MOTA	1479	0	PRO	227 228	35.140 35.535	-7.911 -10 132	0.062 0.346	1.00	0.00	3A7
ATOM ATOM	1480 1481	N CA	PHE	228	36.792		1.060	1.00	0.00	3A7
ATOM	1482	СВ	PHE	228	37.130		1.926	1.00	0.00	3A7
ATOM	1483	CG	PHE	228	37.053		1.172	1.00	0.00	3A7
ATOM	1484	CD1		228	35.821		0.937	1.00	0.00	3A7 3A7
ATOM	1485	CD2		228	38.217 35.753		0.733 0.257	1.00	0.00	3A7
ATOM	1486 1487	CE1		228 228	38.152		0.053	1.00	0.00	3A7
ATOM ATOM	1488	CZ	PHE	228	36.919		-0.187	1.00	0.00	3A7
ATOM	1489	C	PHE	228	37.924	-9.676	0.107	1.00	0.00	3A7
MOTA	1490	0	PHE	228		-10.488		1.00	0.00	3A7 3A7
ATOM	1491	N	LEU	229	38.440 39.469	-8.432 -7.914	0.225 -0.636	1.00	0.00	3A7
ATOM ATOM	1492 1493	CA CB	LEU	229 229	38.924	-7.440	-2.010	1.00	0.00	3A7
ATOM	1494	CG	LEU	229	39.979	-6.871	-2.990	1.00	0.00	3A7
ATOM	1495	CD1		229	41.083	-7.892	-3.326	1.00	0.00	3A7
MOTA	1496	CD2	LEU	229	39.305	-6.347	-4.273	1.00	0.00	3A7
ATOM	1497	C	LEU	229	40.062	-6.752	0.105 0.226	1.00	0.00	3A7 3A7
ATOM	1498 1499	И О	LEU Thr	229 230	41.281 39.186	-6.639 -5.847	0.226	1.00	0.00	3A7
ATOM ATOM	1500	CA	THR	230	39.568	-4.636	1.308	1.00	0.00	3A7
ATOM	1501	СВ	THR	230	38.715	-3.444	0.870	1.00	0.00	3A7
MOTA	1502		THR	230	39.184	-2.215	1.417	1.00	0.00	3A7
ATOM	1503		THR	230	37.220	-3.639	1.206 2.807	1.00	0.00	3A7 3A7
ATOM	1504 1505	C O	THR THR	230 230	39.476 38.513	-4.902 -5.527	3.250	1.00	0.00	3A7
ATOM ATOM	1506	N	PRO	231	40.435	-4.450	3.626	1.00	0.00	3A7
ATOM	1507	CA	PRO	231	40.382	-4.534	5.074	1.00	0.00	3A7
ATOM	1508	CD	PRO	231	41.737	-3.996	3.151	1.00	0.00	3A7
ATOM	1509	CB	PRO	231	41.866	-4.556	5.472 4.409	1.00	0.00	3A7 3A7
ATOM ATOM	1510 1511	CG C	PRO PRO	231 231	42.555 39.661	-3.696 -3.313	5.625	1.00	0.00	3A7
ATOM	1512	ŏ.	PRO	231	38.946	-2.637	4.885	1.00	0.00	3A7
ATOM	1513	N	ILE	232	39.877	-3.024	6.939	1.00	0.00	3A7
ATOM	1514	CA	ILE	232	39.462	-1.870	7.738	1.00	0.00	3A7 3A7
ATOM	1515	CB	ILE	232	40.410 40.450	-0.663 -0.093	7.563 6.123	1.00	0.00	3A7
ATOM ATOM	1516 1517		ILE	232 232	40.186	0.463	8,608	1.00	0.00	3A7
ATOM	1518	CD	ILE	232	40.563	0.068	10.038	1.00	0.00	3A7
ATOM	1519	С	ILE	232	37.983	-1.493	7.610	1.00	0.00	3A7
ATOM	1520	0	ILE	232	37.631	-0.517	6.949	1.00	0.00	3A7 3A7
ATOM	1521	N	LEU	233	37.047	-2.244	8.259	1.00	0.00	3A7
ATOM ATOM	1522 1523	CA CB	LEU	233 233	37.231 36.638	-3.488 -3.490	8.977 10.418	1.00	0.00	3A7
ATOM	1524	CG	LEU	233	37.361	-2.613	11.475	1.00	0.00	3A7
ATOM	1525		LEU	233	38.832	-3.029	11.668	1.00	0.00	3A7
ATOM	1526		LEU	233	37.198	-1.098	11.249	1.00	0.00	3A7 3A7
ATOM	1527	C	LEU	233 233	36.518 36.754	-4.523 -4.608	8.138 6.933	1.00	0.00	3A7
ATOM ATOM	1528 1529	O N	LEU GLU	233	35.621	-5.330	8.775	1.00	0.00	3A7
ATOM	1530	CA	GLU	234	34.755	-6.337	8.183	1.00	0.00	3A7
ATOM	1531	CB	GLU	234	33.985	-5.836	6.925	1.00	0.00	3A7
ATOM	1532	CG	GLU	234	32.750	-6.666	6.514	1.00	0.00	3A7 3A7
ATOM	1533	CD	GLU	234 234	33.141 33.797	-7.946 -7.837	5.777 4.707	1.00	0.00	3A7
ATOM ATOM	1534 1535		GLU	234	32.780	-9.048	6.271	1.00	0.00	3A7
ATOM	1536	C	GLU	234	35.545	-7.587	7.877	1.00	0.00	3A7
ATOM	1537	o	GLU	234	36.385	-7.576	6.978	1.00	0.00	3A7
MOTA	1538	N	ALA	235	35.267	-8.681	8.642	1.00	0.00	3A7 3A7
ATOM ATOM	1539 1540	CA CB	ALA ALA	235 235		-10.014 -10.390	8.499 ·7.067	1.00	0.00	3A7
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MOTA	1541	С	ALA	235	37.017	-10.214	9.409	1.00	0.00	3A7
MOTA	1542	0	ALA	235		-11.312	9.899	1.00	0.00	3A7
MOTA	1543	N	LEU	236	37.790	-9.141	9.671	1.00	0.00	3A7 3A7
MOTA	1544	CA	LEU	236 236	38.971 39.828	-9.206 -7.935	10.503 10.361	1.00	0.00	3A7
MOTA MOTA	1545 1546	CB CG	LEU	236	40.242	-7.612	8.906	1.00	0.00	3A7
ATOM	1547	CD1		236	40.964	-6.254	8.836	1.00	0.00	3A7
ATOM	1548	CD2		236	41.094	-8.728	8.272	1.00	0.00	3A7
MOTA	1549	C	LEU	236	38.601	-9.366	11.956	1.00	0.00	3A7
ATOM	1550	0	LEU	236		-10.138	12.697	1.00	0.00 0.00	3A7 3A7
ATOM	1551 1552	N CA	ASN ASN	237 237	37.530 37.020	-8.664 -8.738	12.387 13.741	1.00	0.00	3A7
ATOM ATOM	1553	CB	ASN	237	35.917	-7.685	13.982	1.00	0.00	3A7
ATOM	1554	CG	ASN	237	36.463	-6.273	13.746	1.00	0.00	3A7
MOTA	1555	OD1	ASN	237	35.922	-5.526	12.923	1.00	0.00	3A7
ATOM	1556		ASN	237	37.544	-5.910	14.500	1.00	0.00	3A7 3A7
ATOM	1557	C	ASN	237		-10.107 -10.658	14.022 15.111	1.00	0.00	3A7
ATOM ATOM	1558 1559	N O	ASN ILE	237 238		-10.707	12.979	1.00	0.00	3A7
ATOM	1560	CA	ILE	238		-12.011	13.021	1.00	0.00	3A7
ATOM	1561	СВ	ILE	238	34.447	-12.290	11.743	1.00	0.00	3A7
ATOM	1562		ILE	238		-13.648	11.845	1.00	0.00	3A7
MOTA	1563		ILE	238		-11.141 -10.932	11.432 12.495	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	1564 1565	CD	ILE	238 238		-13.064	13.260	1.00	0.00	3A7
ATOM	1566	Ö	ILE	238		-13.896	14.106	1.00	0.00	3A7
ATOM	1567	N	THR	239	37.422	-13.013	12.556	1.00	0.00	3A7
ATOM	1568	CA	THR	239		-13.929	12.699	1.00	0.00	3A7
ATOM	1569	CB	THR	239		-13.767	11.574	1.00	0.00	3A7 3A7
ATOM	1570 1571		THR	239 239		-13.766 -14.928	10.323 11.571	1.00	0.00	3A7
ATOM ATOM	1572	C	THR	239		-13.773	14.033	1.00	0.00	3A7
ATOM	1573	ō	THR	239		-14.740	14.603	1.00	0.00	3A7
ATOM	1574		VAL	240		-12.555	14.619	1.00	0.00	3A7
ATOM	1575	CA	VAL	240		-12.276	15.932	1.00	0.00	3A7 3A7
ATOM ATOM	1576 1577	CB	VAL VAL	240 240		-10.784 -10.421	16.162 17.627	1.00	0.00	3A7
ATOM	1578		VAL	240		-10.316	15.239	1.00	0.00	3A7
ATOM	1579	c	VAL	240		-12.842	17.025	1.00	0.00	3A7
MOTA	1580	0	VAL	240		-13.460	17.956	1.00	0.00	3A7
ATOM	1581	N	PHE	241		-12.667	16.920 17.837	1.00	0.00	3A7 3A7
ATOM ATOM	1582 1583	CA .CB	PHE	241 241		-13.266 -12.893	17.483	1.00	0.00	3A7
ATOM	1584	CG	PHE	241		-14.041	17.098	1.00	0.00	. 3A7
MOTA	1585	CD1		241	33.928	-15.104	17.973	1.00	0.00	3A7
ATOM	1586	CD2		241		-14.250	15.746	1.00	0.00	3A7 3A7
ATOM	1587 1588	CE1	PHE	241 241		-16.400 -15.545	17.483 15.244	1.00	0.00	3A7
ATOM ATOM	1589	ÇZ	PHE	241		-16.626	16.119	1.00	0.00	, 3A7
ATOM	1590	Ċ	PHE	241		-14.763	17.938	1.00	0.00	3 <b>A</b> 7
ATOM	1591	0	PHE	241		-15.276	19.050	1.00	0.00	3A7
ATOM	1592	N	PRO	242		-15.511	16.814	1.00	0.00	3A7 3A7
ATOM ATOM	1593 1594	CA CD	PRO	242 242		-16.902 -15.196	16.784 15.686	1.00	0.00	3A7
ATOM	1595	СВ	PRO	242		-17.375	15.333	1.00	0.00	3A7
ATOM	1596	CG	PRO	242	37.313	-16.221	14.553	1.00	0.00	3A7
MOTA	1597	С	PRO	242		-17.310	17.435	1.00	0.00	3A7
MOTA	1598	0	PRO	242		-18.268 -16.603	18.191 17.262	1.00	0.00	3A7 3A7
ATOM ATOM	1599 1600	N CA	ARG ARG	243 243		-16.892	17.893	1.00	0.00	3A7
ATOM	1601	CB	ARG	243		-15.942	17.355	1.00	0.00	3A7
ATOM	1602	CG	ARG	243		-16.265	15.917	1.00	0.00	3A7
MOTA	1603	CD	ARG	243		-15.187	15.348	1.00	0.00	3A7 3A7
ATOM	1604	NE CZ	ARG	243		-15.532 -14.651	13.927 13.096	1.00	0.00	3A7
ATOM ATOM	1605 1606	CZ NH1	ARG	243 243		-14.651	11.800	1.00	0.00	3A7
ATOM	1607		ARG	243		-13.422	13.549	1.00	0.00	3A7
MOTA	1608	С	ARG	243		-16.769	19.398	1.00	0.00	3A7
ATOM	1609	0	ARG	243		-17.580	20.122	1.00	0.00	3A7 3A7
ATOM	1610	N CA	LYS LYS	244 244		-15.774 -15.565	19.905 21.327	1.00	0.00	. 3A7
MOTA MOTA	1611 1612	CB	LYS	244		-14.178	21.648	1.00	0.00	3A7

ATOM	1613	CG	LYS	244	39.241	-13.772	23.119	1.00	0.00	3A7
MOTA	1614	CD	LY\$	244	39.058		23.402		0.00	3A7
MOTA	1615	CE	LYS	244	40.110		22.745	1.00	0.00	3A7
MOTA	1616	NZ	LYS	244	41.474		23.205	1.00	0.00	3A7 3A7
ATOM	1617	C	LYS	244 244	38.844 39.175		21.965 23.051	1.00	0.00	3A7
ATOM ATOM	1618 1619	O N	LYS VAL	244	37.806		21.259	1.00	0.00	3A7
ATOM	1620	CA	VAL	245	37.014		21.692	1.00	0.00	3A7
ATOM	1621	СВ	VAL	245	35.821		20.774	1.00	0.00	3A7
ATOM	1622	CG1	VAL	245		-19.885	21.138	1.00	0.00	3A7
MOTA	1623		VAL	245		-17.368	20.861	1.00	0.00	3A7
ATOM	1624	C	VAL	245		-19.581	21.753 22.748	1.00	0.00 0.00	3A7 3A7
ATOM	1625	0	VAL ILE	245 246		-20.306 -19.822	20.690	1.00	0.00	3A7
MOTA MOTA	1626 1627	N CA	ILE	246		-20.965	20.600	1.00	0.00	3A7
ATOM	1628	CB	ILE	246		-21.026	19.232	1.00	0.00	3A7
ATOM	1629		ILE	246	41.696	-21.593	19.259	1.00	0.00	3A7
ATOM	1630	CG1	ILE	246		-21.855	18.224	1.00	0.00	3A7
MOTA	1631	CD	ILE	246		-21.241	17.793	1.00	0.00	3A7 3A7
ATOM	1632	C	ILE	246		-20.966 -21.996	21.724 22.332	1.00	0.00	3A7
ATOM ATOM	1633 1634	O N	ILE SER	246 247		-19.787	22.059	1.00	0.00	3A7
ATOM	1635	CA	SER	247		-19.652	23.098	1.00	0.00	3A7
ATOM	1636	СВ	SER	247		-18.250	23.119	1.00	0.00	3A7
ATOM	1637	OG	SER	247		-18.000	21.903	1.00	0.00	3A7
ATOM	1638	C	SER	247		-19.917	24.461	1.00	0.00	3A7
ATOM	1639	0	SER	247		-20.579	25.271	1.00	0.00	3A7 3A7
MOTA	1640	N	PHE	248 248		-19.434 -19.654	24.749 26.022	1.00	0.00	3A7
ATOM ATOM	1641 1642	CA CB	PHE	248		-18.900	26.125	1.00	0.00	3A7
ATOM	1643	CG	PHE	248		-17.473	26.559	1.00	0.00	3A7
ATOM	1644		PHE	248		-16.425	25.828	1.00	0.00	. 3A7
ATOM	1645	CD2	PHE	248		-17.176	27.745	1.00	0.00	3A7
MOTA	1646		PHE	248		-15.111	26.274	1.00	0.00	3A7
MOTA	1647		PHE	248		-15.861	28.183	1.00	0.00	3A7 3A7
ATOM ATOM	1648 1649	CZ C	PHE	248 248		-14.827 -21.122	27.447 26.244	1.00	0.00	3A7
ATOM	1650	o	PHE	248		-21.663	27.323	1.00	0.00	3A7
ATOM	1651	N	LEU	249		-21.832	25.198	1.00	0.00	3A7
ATOM	1652	CA	LEU	249	38.585	-23.234	25.317	1.00	0.00	3A7
ATOM	1653	CB	LEU	249		-23.699	24.147	1.00	0.00	3A7
ATOM	1654	CG	LEU	249		-22.962	24.103	1.00	0.00	3A7 3A7
ATOM	1655		LEU	249 249		-23.308 -23.243	22.821 25.342	1.00	0.00	3A7
ATOM ATOM	1656 1657	C	LEU .	249		-24.111	25.396	1.00	0.00	3A7
ATOM	1658	ŏ	LEU	249		-25.088	26.140	1.00	0.00	3A7
ATOM	1659	N	THR	250		-23.744	24.670	1.00	0.00	3A7
ATOM	1660	CA	THR	250		-24.464	24.706	1.00	0.00	3A7
ATOM .	1661	CB	THR	250		-23.926	23.673	1.00	0.00	3A7
MOTA	1662		THR	250		-24.120	22.372	1.00	0.00	3A7 3A7
ATOM	1663		THR	250 250		-24.649 -24.398	23.731 26.085	1.00	0.00	3A7
ATOM ATOM	1664 1665	С 0	THR THR	250		-25.376	26.573	1.00	0.00	3A7
ATOM	1666	N	LYS	251		-23.243	26.777	1.00	0.00	3A7
ATOM	1667	CA	LYS	251	43.087	-23.060	28.132	1.00	0.00	3A7
MOTA	1668	CB	LYS	251		-21.601	28.592	1.00	0.00	3A7
MOTA	1669	CG	LYS	251		-21.282	29.945	1.00	0.00	3A7 3A7
ATOM ATOM	1670	CD	LYS LYS	251 251		-19.803 -19.494	30.335 31.700	1.00	0.00	3A7
MOTA	1671 1672	NZ	LYS	251		-18.062	32.038	1.00	0.00	3A7
ATOM	1673	c	LYS	251		-23.933	29.091	1.00	0.00	3A7
ATOM	1674	ō	LYS	251		-24.559	29.945	1.00	0.00	3A7
MOTA	1675	N	SER	252		-24.057	28.942	1.00	0.00	3A7
MOTA	1676	CA	SER	252		-24.912	29.776	1.00	0.00	3A7
MOTA	1677	CB	SER	252		-24.780	29.422	1.00	0.00	3A7 3A7
MOTA	1678 1679	oG C	SER	252 252		-23.431 -26.371	29.562 29.662	1.00	0.00	3A7
ATOM ATOM	1680	0	SER SER	252		-27.089	30.653	1.00	0.00	3A7
MOTA	1681	N	VAL	253		-26.832	28.425	1.00	0.00	3A7
ATOM	1682	CA	VAL	253	41.211	-28.203	28.125	1.00	0.00	3A7
MOTA	1683	CB	VAL	253		-28.416	26.609	1.00	0.00	3A7
MOTA	1684	CG1	VAL	253	41.865	-29.803	26.237	1.00	0.00	3A7

ATOM	1685	CG2	VAL	253	39.8	86 -28.264	25.997	1.00	0.00	3A7
ATOM	1686	c	VAL	253		32 -28.553		1.00	0.00	3A7
ATOM	1687	ŏ	VAL	253		84 -29.586		1.00	0.00	3A7
	-	N	LYS	254		18 -27.644		1.00	0.00	3A7
ATOM	1688					42 -27.794		1.00	0.00	3A7
ATOM	1689	CA	LYS	254				1.00	0.00	3A7
ATOM	1690	СВ	LYS	254		35 -26.640				3A7
ATOM	1691	CG	LYS	254		20 -26.788		1.00	0.00	3A7
MOTA	1692	CD	LYS	254		43 -25.705		1.00	0.00	
MOTA	1693	CE	LYS	254		79 -24.338		1.00	0.00	3A7
ATOM	1694	NZ	LYS	254		11 -23.622		1.00	0.00	3A7
ATOM	1695	С	LYS	254		30 -27.834		1.00	0.00	3A7
ATOM	1696	0	LYS	254	45.4	12 -28.728	31.270	1.00	0.00	3A7
MOTA	1697	N	GLN	255	44.0	98 -26.892	31.313	1.00	0.00	3A7
ATOM	1698	CA	GLN	255	43.9	43 -26.855	32.753	1.00	0.00	3A7
MOTA	1699	СВ	GLN	255	43.1	22 -25.635	33.238	1.00	0.00	3A7
ATOM	1700	CG	GLN	255		63 -24.302		1.00	0.00	3A7
ATOM	1701	CD	GLN	255		77 -23.153		1.00	0.00	3A7
	1702		GLN	255		32 -22.444		1.00	0.00	3A7
ATOM		NE2		255		01 -22.974		1.00	0.00	3A7
ATOM	1703					83 -28.104		1.00	0.00	3A7
ATOM	1704	C	GLN	255				1.00	0.00	3A7
ATOM	1705	0	GLN	255		99 -28.568			0.00	3A7
ATOM	1706	И	ILE	256		75 -28.710		1.00		3A7
ATOM	1707	CA	ILE	256		79 -29.907		1.00	0.00	
ATOM	1708	CB	ILE	256		04 -30.098		1.00	0.00	3A7
ATOM	1709	CG2	ILE	256		68 -31.597		1.00	0.00	3A7
ATOM	1710	CG1	ILE	256		.98 -29.508		1.00	0.00	3A7
MOTA	1711	CD	ILE	256		70 -28.036		1.00	0.00	3A7
ATOM	1712	С	ILE	256	42.5	66 -31.136	32.826	1.00	0.00	3A7
MOTA	1713	0	ILE	256	42.4	11 -32.060	33.627	1.00	0.00	3A7
ATOM	1714	N	LYS	257	43.5	35 -31.169	31.881	1.00	0.00	3A7
ATOM	1715	CA	LYS	257	44.4	64 -32.272	31.759	1.00	0.00	3A7
ATOM	1716	CB	LYS	257	45.2	16 -32.240	30.418	1.00	0.00	3A7
ATOM	1717	CG	LYS	257		04 -32.548		1.00	0.00	3A7
ATOM	1718	CD	LYS	257		27 -32.67		1.00	0.00	3A7
ATOM	1719	ČE	LYS	257		83 -31.36		1.00	0.00	3A7
	1720	NZ	LYS	257		99 -30.90		1.00	0.00	3A7
ATOM	1721	C	LYS	257		89 -32.28		1.00	0.00	3A7
ATOM						44 -33.34		1.00	0.00	3A7
MOTA	1722	0	LYS	257				1.00	0.00	3A7
ATOM	1723	N	GLU	258		356 -31.08		1.00	0.00	3A7
ATOM	1724	CA	GLU	258		317 -30.92			0.00	3A7
ATOM	1725	СВ	GLU	258		154 -29.51		1.00		3A7
ATOM	1726	CG	GLU	258		42 -29.21		1.00	0.00	
ATOM	1727	CD	GLU	258		02 -30.19		1.00	0.00	3A7
MOTA	1728		GLU	258		86 -30.20		1.00	0.00	3A7
ATOM	1729	OE2	GLU	258		118 -30.95		1.00	0.00	3A7
MOTA	1730	С	GLU	258		74 -31.15		1.00	0.00	3A7
ATOM	1731	0	GLU	258	46.8	351 -31.50	1 36.763	1.00	0.00	3A7
ATOM	1732	N	GLY	259	44.8	29 -30.97	1 35.870	1.00	0.00	3A7
ATOM	1733	CA	GLY	259	44.0	26 -31.19	4 37.052	1.00	0.00	3A7
ATOM	1734		GLY	259	43.4	90 -32.59	8 37.051	1.00	0.00	3A7
ATOM	1735	0	GLY	259	44.0	04 -33.46	1 36.340	1.00	0.00	3A7
ATOM	1736	N	ARG	260	42.4	144 -32.84	2 37.887	1.00	0.00	3A7
ATOM	1737	CA	ARG	260	41.7	787 -34.11	8 38.133	1.00	0.00	3A7
ATOM	1738	СВ	ARG	260		189 -34.95		1.00	0.00	3A7
ATOM	1739	CG	ARG	260		39 -36.23		1.00	0.00	3A7
ATOM	1740	CD	ARG	260		72 -36.00		1.00	0.00	3A7
				260		05 -35.66		1.00	0.00	3A7
ATOM	1741	NE	ARG			949 -35.26		1.00	0.00	3A7
ATOM	1742	CZ	ARG	260						3A7
ATOM	1743		ARG	260		967 -34.92		1.00	0.00	3A7
MOTA	1744		ARG	260		784 -35.17		1.00	0.00	
MOTA	1745	С	ARG	260		531 -34.89		1.00	0.00	3A7
MOTA	1746	0	ARG	260		344 -35.83		1.00	0.00	3A7
MOTA	1747	N	LEU	261		81 -34.47		1.00	0.00	3A7
ATOM	1748	CA	LEU	261		173 -34.94		1.00	0.00	3A7
ATOM	1749	СВ	LEU	261	44.4	163 -33.85		1.00		3A7
MOTA	1750	CG	LEU	261	43.8	383 -32.58		1.00	0.00	3A7
ATOM	1751	CD1	LEU	261	45.0	023 -31.73	7 43.230	1.00		3A7
ATOM	1752		LEU	261	43.0	009 -31.70	8 41.709	1.00	0.00	3A7
ATOM	1753	C	LEU	261		675 -35.51				3A7
ATOM	1754	ō	LEU	261		042 -36.54		1.00	0.00	3A7
ATOM	1755	N	LYS	262		569 -34.83				3A7
ATOM	1756	CA	LYS	262		788 -35.23				3A7
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ATOM	1757	СВ	LYS	262	41.421	-34.790	45.462	1.00	0.00	3A7
ATOM	1758	CG	LYS	262	40.810		46.708	1.00	0.00	3A7
ATOM	1759	CD	LYS	262	41.515	-35.043	48.009	1.00	0.00	3A7
ATOM	1760	CE	LYS	262	41.066		49.233	1.00	0.00	3A7
ATOM	1761	NZ	LYS	262	39.611		49.468	1.00	0.00	3A7
ATOM	1762	С	LYS	262	39.442		43.941	1.00	0.00	3A7
MOTA	1763	0	LYS	262	39.325		43.313	1.00	0.00	3A7 3A7
MOTA	1764	N	GLU	263	38.381		44.510	1.00	0.00	3A7
MOTA	1765	CA	GLU	263	37.009		44.438 44.396	1.00	0.00	3A7
ATOM	1766	CB CG	GTN GTN	263 263	36.001 36.178		43.152	1.00	0.00	3A7
MOTA MOTA	1767 1768	CD	GLU	263	35.147		43.149	1.00	0.00	3A7
ATOM	1769		GLU	263	34.322		44.098	1.00	0.00	3A7
ATOM	1770		GLU	263	35.174		42.183	1.00	0.00	3A7
ATOM	1771	С	GLU	263	36.698	-33.900	45.630	1.00	0.00	3A7
MOTA	1772	٥	GLU	263	35.910		46.501	1.00	0.00	3A7
ATOM	1773	N	THR	264		-32.704	45.670	1.00	0.00	3A7
MOTA	1774	CA	THR	264	37.170		46.715	1.00	0.00	3A7 3A7
ATOM	1775	CB	THR	264	38.280	-31.765	47.757 48.352	1.00	0.00	3A7
ATOM	1776		THR	264	38.047		48.870	1.00	0.00	3A7
ATOM	1777	CGZ	THR THR	264 264		-30.395	46.003	1.00	0.00	3A7
ATOM ATOM	1778 1779	ŏ	THR	264		-29.458	46.415	1.00	0.00	3A7
ATOM	1780	N	GLN	265		-30.300	44.890	1.00	0.00	3A7
ATOM	1781	CA	GLN	265	38.063	-29.123	44.052	1.00	0.00	3A7
ATOM	1782	СВ	GLN	265	39.417	-29.038	43.298	1.00	0.00	3A7
MOTA	1783	CG	GLN	265		-28.808	44.201	1.00	0.00	3A7
MOTA	1784	CD	GLN	265		-30.055	45.032	1.00	0.00	3A7 3A7
MOTA	1785		GLN	265		-31.165	44.497	1.00	0.00	3A7
ATOM	1786		GLN	265		-29.849 -29.140	46.374	1.00	0.00	3A7
ATOM	1787	С 0	GLN GLN	265 265		-28.132	42.802	1.00	0.00	3A7
ATOM ATOM	1788 1789	N	LYS	266		-30.320	42.404	1.00	0.00	3A7
ATOM	1790	CA	LYS	266		-30.556	41.500	1.00	0.00	3A7
ATOM	1791	СВ	LYS	266	36.035	-30.452	40.002	1.00	0.00	3A7
ATOM	1792	CG	LYS	266	37.305	-31.216	39.591	1.00	0.00	3A7
MOTA	1793	CD	LYS	266		-30.959	38.129	1.00	0.00	3A7
ATOM	1794	CE	LYS	266		-31.700	37.724	1.00	0.00	3A7 3A7
MOTA	1795	NZ	LYS	266		-31.401	36.320	1.00	0.00	3A7
ATOM	1796	C	LYS	266		-31.922 -32.934	41.858 41.655	1.00	0.00	3A7
ATOM ATOM	1797 1798	O N	LYS HIS	266 267		-31.966	42.437	1.00	0.00	3A7
ATOM	1799	CA	HIS	267		-33.168	42.940	1.00	0.00	3A7
ATOM	1800		HIS	267		-35.052	45.499	1.00	0.00	3A7
ATOM	1801	CG	HIS	267	31.780	-34.098	44.815	1.00	0.00	3A7
ATOM	1802	СB	HIS	267		-32.874	44.174	1.00	0.00	3A7
ATOM	1803		HIS	267		-35.724	45.524	(1.00	0.00	3A7
ATOM	1804		HIS	267	. 30.489		44.840	1.00	0.00	3A7 3A7
MOTA	1805		HIS	. 267		-35.999 -33.802	45,901 41.858	1.00	0.00	3A7
ATOM	1806 1807	С 0	HIS HIS	267 267		-35.018	41.834	1.00	0.00	3A7
ATOM ATOM	1808	N	ARG	268		-32.963	40.929	1.00	0.00	3A7
ATOM	1809	CA	ARG	268		-33.390	39.804	1.00	0.00	3A7
MOTA	1810	СВ	ARG	268	29.939	-32.419	39.501	1.00	0.00	3A7
ATOM	1811	CG	ARG	268		-30.974	39.172	1.00	0.00	3A7
MOTA	1812	CD	ARG	268		-30.049	38.948	1.00	0.00	3A7
ATOM	1813	NE	ARG	268		-28.690	38.573	1.00	0.00	3A7 3A7
ATOM	1814	CZ	ARG	268		-27.637	38.353	1.00	0.00	3A7 3A7
ATOM	1815		ARG	268 268		-26.423 -27.791	37.993 38.491	1.00	0.00	3A7
ATOM	1816		ARG ARG	268		-33.501	38.593	1.00	0.00	3A7
ATOM ATOM	1817 1818	C O	ARG	268		-32.813	38.485	1.00	0.00	3A7
ATOM	1819	N	VAL	269		-34.383	37.643	1.00	0.00	3A7
ATOM	1820	CA	VAL	269		-34.566	36.378	1.00	0.00	3A7
ATOM	1821	СВ	VAL	269		-36.021	36.063	1.00	0.00	3A7
ATOM	1822		VAL	269		-36.473	37.001	1.00	0.00	3A7
MOTA	1823		VAL	269		-36.903	36.220	1.00	0.00	3A7 3A7
ATOM	1824	C	VAL	269		-33.947	35.315	1.00	0.00	3A7
ATOM	1825	0	VAL	269 270		-33.712 -33.642	35.519 34.156	1.00	0.00	3A7
ATOM ATOM	1826 1827	N CA	ASP ASP	270	32.030		33.096	1.00	0.00	3A7
ATOM	1828	CB	ASP	270		-31.399	33.132	1.00	0.00	3A7

ATOM	1829	CG	ASP	270	33.510 -	31.368	33.034	1.00	0.00	3A7
ATOM	1830		ASP	270	34.013 -	30.868	31.995	1.00	0.00	3A7
ATOM	1831	OD2	ASP	270	34.191 -	31.809	33.998	1.00	0.00	3A7
MOTA	1832	С	ASP	270	31.710 -		31.781	1.00	0.00	3A7
MOTA	1833	0	ASP	270	32.369 -		31.709	1.00	0.00	3A7
ATOM	1834	Ŋ	PHE	271	31.187 -		30.684	1.00	0.00	3A7 3A7
ATOM	1835	CA	PHE	271	31.302 -		29.357	1.00	0.00 0.00	3A7
MOTA	1836	CB	PHE	271	30.407 -		28.356 27.080	1.00	0.00	3A7
ATOM	1837	CG	PHE	271 271	30.344 -: 30.012 -:		27.101	1.00	0.00	3A7
MOTA MOTA	1838 1839		PHE	271	30.758 -		25.887	1.00	0.00	3A7
ATOM	1840		PHE	271	30.211 -		25.972	1.00	0.00	3A7
ATOM	1841		PHE	271	30.870 -		24.737	1.00	0.00	3A7
ATOM	1842	CZ	PHE	271	30.646 -		24.793	1.00	0.00	3A7
ATOM	1843	C	PHE	271	32.719 -	33.478	28.848	1.00	0.00	3A7
ATOM	1844	0	PHE	271	33.150 -		28.204	1.00	0.00	3A7
MOTA	1845	N	LEU	272	33.494 -		29.146	1.00	0.00	3A7
MOTA	1846	CA	LEU	272	34.866 -		28.716	1.00	0.00	3A7
MOTA	1847	CB	LEU	272	35.455 -		29.100	1.00	0.00	3A7 3A7
MOTA	1848	CG	LEU	272	36.816 -		28.482	1.00	0.00	3A7
ATOM	1849		LEU	272	36.864 - 38.027 -		28.078 29.363	1.00	0.00	3A7
ATOM	1850	CDZ	LEU LEU	272 272	35.735 -		29.311	1.00	0.00	3A7
ATOM ATOM	1851 1852	Ö	LEU	272	36.573 -		28.634	1.00	0.00	3A7
ATOM	1853	N	GLN	273	35.522 -		30.606	1.00	0.00	3A7
ATOM	1854	CA	GLN	273	36.255 -		31.288	1.00	0.00	3A7
ATOM	1855	СВ	GLN	273	35.890 -		32.788	1.00	0.00	3A7
ATOM	1856	CG	GLN	273	36.853 -	35.634	33.658	1.00	0.00	3A7
ATOM	1857	CD	GLN	273	38.222 -	34.946	33.686	1.00	0.00	3A7
MOTA	1858		GLN	273	38.361 -		34.234	1.00	0.00	3A7
ATOM	1859		GLN	273	39.247 -		33.079	1.00	0.00	3A7
ATOM	1860	C	GLN	273	35.971 -		30.668	1.00	0.00	3A7 3A7
ATOM	1861	0	GLN	273	36.882 -		30.456 30.310	1.00	0.00	3A7
ATOM	1862	N	LEU	274 274	34.685 - 34.245 -		29.669	1.00	0.00	3A7
ATOM	1863 1864	CA CB	LEU	274	32.718 -		29.471	1.00	0.00	3A7
ATOM ATOM	1865	CG	LEU	274	31.891 -		30.761	1.00	0.00	3A7
ATOM	1866		LEU	274	30.398 -		30.394	1.00	0.00	3A7
ATOM	1867		LEU	274	32.273 -		31.558	1.00	0.00	3A7
ATOM	1868	С	LEU	274	34.854 -	37.729	28.302	1.00	0.00	3A7
ATOM	1869	0	LEU	274	35.232 -	38.832	27.930	1.00	0.00	3A7
ATOM	1870	N	MET	275	35.003 -		27.521	1.00	0.00	3A7
ATOM	1871	CA	MET	275	35.607 -		26.211	1.00	0.00	3A7
ATOM .		CB	MET	275	35.400 -		25.399	1.00	0.00	3A7 3A7
ATOM	1873	CG	MET	275	33.958 -		24.962 23.713	1.00	0.00	3A7
ATOM ATOM	1874	.SD CE	MET MET	275 275	33.857 - 34.315 -		24.786	1.00	0.00	3A7
ATOM	1875 1876	C	MET	275	37.090 -		26.286	1.00	0.00	3A7
ATOM	1877	Q	MET	275	37.642 -		25.458	1.00	0.00	. 3A7
ATOM	1878	Ŋ	ILE	276	37.778 -		27.305	1.00	0.00	3A7
ATOM	1879	CA	ILE	276	39.215 -		27.488	1.00	0.00	3A7
ATOM	1880	СВ	ILE	276	39.723 -	35.567	28.575	1.00	0.00	3A7
ATOM	1881	CG2	ILE	276	41.140 -	35.906	29.105	1.00	0.00	3A7
MOTA	1882	CG1	ILE	276	39.717 -		28.081		0.00	3A7
MOTA	1883	CD	ILE	276	40.767 -		27.011	1.00	0.00	3A7
ATOM	1884	Ç	ILE	276	39.615 -		27.833 27.476	1.00	0.00	3A7 3A7
ATOM	1885	0	ILE	276	40.701 - 38.749 -		28.548	1.00	0.00	3A7
ATOM	1886	N	ASP ASP	277 277	39.133 -		29.016	1.00	0.00	3A7
MOTA MOTA	1887 1888	CA CB	ASP	277	38.914 -		30.516	1.00	0.00	3A7
ATOM	1889	CG	ASP	277	39.827 -		31.302	1.00	0.00	3A7
ATOM	1890		ASP	277	40.999 -		30.882	1.00	0.00	3A7
ATOM	1891		ASP	277	39.351 -		32.329	1.00	0.00	3A7
ATOM	1892	С	ASP	277	38.346 -	41.070	28.476	1.00	0.00	3A7
ATOM	1893	0	ASP	277	38.933 -		28.164	1.00	0.00	3A7
ATOM	1894	N	SER	278	36.987 -		28.602	1.00	0.00	3A7
MOTA	1895	CA	SER	278	36.186 -		29.071	1.00	0.00	3A7
MOTA	1896	CB	SER	278	34.677 -		29.196	1.00	0.00	3A7 3A7
MOTA	1897	OG	SER	278	34.091 -		27.961	1.00	0.00	3A7
MOTA	1898	C	SER	278	36.329 - 35.567 -		28.318 27.399	1.00	0.00	3A7
MOTA	1899	0	SER	278 279	35.367 - 37.341 -		28.750	1.00	0.00	3A7
MOTA	1900	N	GLN	213	37.341	17.30/	20.750	2.00		

ATOM	1901	CA	GLN	279	37.851 -45.5	39 28.167	1.00	0.00	3A7
ATOM	1902	СВ	GLN	279	36.793 -46.5	03 27.561	1.00	0.00	3A7
ATOM	1903	CG	GLN	279	35.768 -47.0	00 28.593	1.00	0.00	3A7
ATOM	1904	CD	GLN	279	34.775 -47.9	28 27.887	1.00	0.00	3A7
ATOM	1905		GLN	279	35.143 -49.0		1.00	0.00	3A7
ATOM	1906	NE2		279	33.487 -47.4		1.00	0.00	3 <b>A</b> 7
ATOM	1907	c	GLN	279	38.889 -45.2		1.00	0.00	3A7
	1908	ŏ	GLN	279	38.687 -45.4		1.00	0.00	. 3A7
ATOM				280	40.027 -44.5			0.00	3A7
ATOM	1909	N	ASN	280	41.202 -44.1		1.00	0.00	3A7
ATOM	1910	CA	ASN		42.008 -45.3		1.00	0.00	3A7
ATOM	1911	CB	ASN	280	42.430 -46.2		1.00	0.00	3A7
ATOM	1912	CG	ASN	280			1.00	0.00	3A7
MOTA	1913		ASN	280	41.937 -47.4		1.00	0.00	3A7
MOTA	1914		ASN	280	43.366 -45.8				3A7
ATOM	1915	С	ASN	280	40.890 -43.1		1.00	0.00	3A7 ·
MOTA	1916	0	ASN	280	40.934 -43.5		1.00	0.00	
ATOM	1917	N	SER	281	40.551 -41.9		1.00	0.00	3A7
ATOM	1918	CA	SER	281	40.076 -40.8		1.00	0.00	3A7
ATOM	1919	СВ	SER	281	40.924 -40.5		1.00	0.00	3A7
ATOM	1920	OG	SER	281	42.283 -40.2		1.00	0.00	3A7
ATOM	1921	С	SER	281	38.621 -40.9		1.00	0.00	3A7
ATOM	1922	0	SER	281	38.131 -40.1	72 24.021	1.00	0.00	3A7
ATOM	1923	N	LYS	282 .	37.924 -42.0	20 25.342	1.00	0.00	3A7
MOTA	1924	CA	LYS	282	36.818 -42.7	23 24.707	1.00	0.00	3A7
ATOM	1925	СВ	LYS	282	35.459 -42.0	13 24.620	1.00	0.00	3A7
ATOM	1926	CG	LYS	282	34.288 -42.9	57 24.294	1.00	0.00	3A7
ATOM	1927		LYS	282	32.914 -42.3	36 24.590	1.00	0.00	3A7
ATOM	1928	CE	LY\$	282	31.744 -43.3	01 24.357	1.00	0.00	3A <b>7</b>
ATOM	1929	NZ	LYS	282	31.691 -43.7		1.00	0.00	3A7
ATOM	1930	С	LYS	282	37.194 -43.1		1.00	0.00	3A7
ATOM	1931	ō	LYS	282	37.082 -42.4		1.00	0.00	3A7
ATOM	1932	N	ASP	283	37.706 -44.3		1.00	0.00	3A7
ATOM	1933	CA	ASP	283	38.125 -44.9		1.00	0.00	3A7
ATOM	1934	СВ	ASP	283	39.663 -45.0		1.00	0.00	3A7
ATOM	1935	CG	ASP	283	40.442 -46.0		1.00	0.00	3A7
ATOM	1936		ASP	283	41.683 -46.0		1.00	0.00	3A7
ATOM	1937		ASP	283	39.853 -46.6		1.00	0.00	3A7
ATOM	1938	C	ASP	283	37.352 -46.2		1.00	0.00	3A7
ATOM	1939	Ö	ASP	283	37.675 -47.2		1.00	0.00	3A7
MOTA	1940	N	SER	284	36.258 -46.1		1.00	0.00	3A7
	1941	CA	SER	284	35.513 -47.3		1.00	0.00	3A7
ATOM	1942		SER	284	34.115 -47.0		1.00	0.00	3A7
ATOM		CB		284	34.183 -45.9		1.00	0.00	3A7
ATOM	1943	og c	SER		36.266 -48.2		1.00	0.00	3A7
MOTA	1944	C	SER	284			1.00	0.00	3A7
MOTA	1945	0	SER	284	36.990 -49.1		1.00	0.00	3A7
ATOM	1946	N	GLU	285	36.113 -48.0		1.00	0.00	3A7
MOTA	1947	CA	GLU	285	36.639 -49.0 35.795 -49.2			0.00	3A7
ATOM	1948	CB	GLU	285			1.00		3A7
	.1949	CG.	GLU	285	35.628 -47.8		1.00	0.00	3A7
ATOM	1950	CD	GLU	285	34.752 -48.1		1.00	0.00	3A7
ATOM	1951		GLU	285	33.566 ~48.5		1.00	0.00	3A7
ATOM	1952		GLU	285	35.255 -47.9		1.00	0.00	
ATOM	1953	С	GLU	285	38.083 -48.8		1.00	0.00	3A7
MOTA	1954	0	GLU	285	38.621 -49.4			0.00	3A7
ATOM	1955	N	THR	286	38.744 -47.9		1.00	0.00	3A7
MOTA	1956	CA	THR	286	40.099 -47.3		1.00	0.00	3A7
MOTA	1957	СВ	THR	286	41.251 -48.3		1.00	0.00	3A7
MOTA	1958		THR	286	41.071 -49.4		1.00	0.00	3A7
MOTA	1959	CG2	THR	286	42.623 -47.7		1.00	0.00	3A7
MOTA	1960	С	THR	286	40.161 -46.3		1.00	0.00	3A7
ATOM	1961	0	THR	286	41.095 -45.5		1.00	0.00	3A7
ATOM	1962	N	HIS	287	39.201 -46.2		1.00	0.00	3A7
ATOM	1963	CA	HIS	287	39.294 -45.5		1.00	0.00	3A7
MOTA	1964	ND1	HIS	287	37.806 -44.4			0.00	3A7
MOTA	1965	CG	HIS	287	38.588 -45.4			0.00	3A7
ATOM	1966	СВ	HIS	287	38.440 -46.1	52 13.541	1.00	0.00	3A7
ATOM	1967		HIS	287	39.260 -44.9	03 10.120	1.00	0.00	3A7
ATOM	1968		HIS	287	39.470 -45.7	56 11.189	1.00	0.00	3A7
MOTA	1969		HIS	287	38.251 -44.1			0.00	3A7
ATOM	1970	C	HIS	287	38.868 -44.1		1.00	0.00	3A7
ATOM	1971	ō	HIS	287	37.679 -43.7		1.00	0.00	3A7
ATOM	1972	N	LYS	288	39.880 -43.2			0.00	3A7
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ATOM	1973	CA	LYS	288	39.776	5 -41.800	15.358	1.00	0.00	3A7
ATOM	1974	СВ	LYS	288		-41.036	14.340	1.00	0.00	3A7
ATOM	1975	CG	LYS	288	39.415	5 -41.157	12.901	1.00	0.00	3A7
ATOM	1976	CD	LYS	288		3 -40.437	11.877	1.00	0.00	3A7
MOTA	1977	CE	LYS	288		5 -40.557	10.434	1.00	0.00	3A7
MOTA	1978	NZ	LYS	288		3 -39.909	10.282	1.00	0.00	3A7
MOTA	1979	C	LYS	288		9 -41.522	16.767	1.00	0.00	3A7 3A7
ATOM	1980	0	LYS	288 289		6 -41.380 3 -41.406	17.030 17.701	1.00	0.00	3A7
MOTA MOTA	1981 1982	N CA	ALA ALA	289		2 -40.977	19.070	1.00	0.00	3A7
ATOM	1983	CB	ALA	289		3 -41.545	20.027	1.00	0.00	3A7
MOTA	1984	c	ALA	289		4 -39.473	19.078	1.00	0.00	3A7
ATOM	1985	ō	ALA	289		-38.875	18.128	1.00	0.00	3A7
ATOM	1986	N	LEU	290	39.624	4 -38.812	20.137	1.00	0.00	3A7
MOTA	1987	CA	LEU	290	39.349	9 -37.401	20.081	1.00	0.00	3A7
MOTA	1988	CB	LEU	290		37.004	21.014	1.00	0.00	3A7
MOTA	1989	CG	LEU	290		3 -37.703	20.701	1.00	0.00	3A7
MOTA	1990		LEU	290		2 -37.512	21.861	1.00	0.00	3A7 3A7
ATOM	1991		LEU	290		2 -37.221	19.355	1.00	0.00	3A7 3A7
ATOM	1992	C	LEU	290 290		) -36.573 l -36.642	20.350 21.390	1.00	0.00	3A7
ATOM ATOM	1993 1994	O N	LEU SER	291		4 -35.731	19.352	1.00	0.00	3A7
ATOM	1995	CA	SER	291		4 -34.822	19.363	1.00	0.00	3A7
ATOM	1996	СВ	SER	291		5 -34.592	17.928	1.00	0.00	3A7
ATOM	1997	OG.	SER	291		2 -34.204	17.030	1.00	0.00	3A7
ATOM	1998	С	SER	291		1 -33.540	19.957	1.00	0.00	3A7
MOTA	1999	0	SER	291		5 -33.273	19.991	1.00	0.00	3A7
MOTA	2000	N	ASP	292		0 -32.681	20.410	1.00	0.00	3A7
ATOM	2001	CA	ASP	292		1 -31.438	21.064	1.00	0.00	3A7 .
MOTA	2002	CB	ASP	292		B -30.745	21.556	1.00	0.00	3A7 3A7
ATOM	2003	CG	ASP	292		2 -31.647 6 -31.941	22.570 23.629	1.00 1.00	0.00	3A7
ATOM	2004 2005		ASP ASP	292 292		4 -32.050	22.298	1.00	0.00	3A7
MOTA MOTA	2005	C	ASP	292		4 -30.471	20.170	1.00	0.00	3A7
ATOM	2007	ŏ	ASP	292	•	8 -29.641	20.643	1.00	0.00	3A7
ATOM	2008	N	LEU	293		6 -30.616	18.834	1.00	0.00	3A7
ATOM	2009	CA	LÈU	293	40.83	6 ~29.795	17.858	1.00	0.00	3A7
ATOM	2010	CB	LEU	293		7 -29.876	16.490	1.00	0.00	3A7
MOTA	2011	CG	LEU	293		1 -29.436	16.506	1.00	0.00	3A7
λтом	2012		LEU	293		3 -29.663	15.129	1.00	0.00	3A7 3A7
ATOM	2013		LEU	293		9 -27.976	16.965	1.00	0.00	3A7
ATOM	2014	C	LEU	293		2 -30.187 3 -29.340	17.711 17.738	1.00	0.00	3A7
ATOM ATOM	2015 2016	N O	LEU GLU	293 294		1 -31.502	17.619	1.00	0.00	3A7
ATOM	2017	CA	GLU	294		2 -31.998	17.504	1.00	0.00	3A7
ATOM	2018	СВ	GLU	294		7 -33.523	17.310	1.00	0.00	3A7
ATOM	2019	CG	GLU	294		7 -33.957	15.942	1.00	0.00	3A7
ATOM	2020	CD	GLU	294		8 -35.480	15.850	1.00	0.00	3A7
MOTA	2021	OE1	GLU	294		0 -36.040	15.905	1.00	0.00	3A7
ATOM	2022		GLU	294		5 -36.104	15.722	1.00	0.00	3A7
ATOM	2023	C	GLU	294		1 -31.676	18.723	1.00	0.00	3A7 3A7
ATOM	2024	0	GLU	294		6 -31.192 6 -31.876	18.632 19.909	1.00	0.00	3A7 3A7
ATOM	2025	N	LEU	295		5 -31.573	21.190	1.00	0.00	3A7
ATOM ATOM	2026 2027	CA CB	LEU	295 295		1 -31.878	22.313	1.00	0.00	3A7
ATOM	2028	CG	LEU	295		1 -33.35B	22.435	1.00	0.00	3A7
ATOM	2029		LEU	295		4 -33.555	23.470	1.00	0.00	3A7
ATOM	2030		LEU	295	37.09	4 -34.206	22.783	1.00	0.00	3A7
MOTA	2031	С	LEU	295		5 -30.119	21.312	1.00	0.00	3A7
ATOM	2032	0	LEU	295		4 -29.765	21.643	1.00	0.00	3A7
MOTA	2033	N	MET	296		8 -29.212	21.017	1.00	0.00	3A7
MOTA	2034	CA	MET	296		5 -27.783	21.050	1.00	0.00	3A7 3A7
MOTA	2035	CB	MET	296		0 -27.070	20.647	1.00	0.00	3A7 3A7
ATOM	2036	CG	MET	296		0 -25.578 6 -24.717	20.350	1.00	0.00	3A7
ATOM ATOM	2037 2038	SD CE	MET MET	296 296		7 <b>-</b> 25.540	18.974	1.00	0.00	3A7
ATOM	2038	CE	MET	296		5 -27.341	20.113	1.00	0.00	3A7
ATOM	2040	õ	MET	296		8 -26.566	20.489	1.00	0.00	3A7
ATOM	2041	N	ALA	297		4 -27.882	18.877	1.00	0.00	3A7
ATOM	2042	CA	ALA	297		2 -27.555	17.895	1.00	0.00	3A7
ATOM	2043	CB	ALA	297		3 -28.182	16.525	1.00	0.00	3A7
ATOM	2044	С	ALA	297	33.78	3 -27.978	18.300	1.00	0.00	3A7

ATOM	2045	0	ALA	297	32.81	7 -27.301	17.986	1.00	0.00	3A7
ATOM	2046	N	GLN	298		B -29.071	19.085	1.00	0.00	3A7
ATOM	2047	CA	GLN	298	32.38	5 -29.501	19.640	1.00	0.00	3A7
MOTA	2048	CB	GLN	298		2 -30.905	20.248	1.00	0.00	3A7
MOTA	2049	CG	GLN	298		1 -32.025	19.207	1.00	0.00	3A7
MOTA	2050	CD	GLN	298		8 -33.345	19.922	1.00	0.00	3A7
MOTA	2051		GLN	298		0 -33.554	20.400	1.00	0.00	3A7
MOTA	2052	NE2	GLN	298		9 -34.253	19.977	1.00	0.00	3A7
ATOM	2053	C	GLN	298		2 -28.563	20.719	1.00	0.00	3A7 3A7
ATOM	2054	0	GLN	298		3 -28.142 1 -28.160	20.728 21.630	1.00	0.00	3A7
ATOM	2055	N	SER	299 299		5 -27.222	22.690	1.00	0.00	3A7
MOTA MOTA	2056 2057	CA CB	SER SER	299		9 -27.023	23.597	1.00	0.00	3A7
ATOM	2058	OG	SER	299		5 -28.269	24.141	1.00	0.00	3A7
ATOM	2059	ç	SER	299		7 -25.874	22.158	1.00	0.00	3A7
ATOM	2060	ŏ	SER	299		5 -25.252	22.698	1.00	0.00	3A7
ATOM	2061	N	ILE	300		9 -25.399	21.047	1.00	0.00.	3 <b>A</b> 7
ATOM	2062	CA	ILE	300	32.36	1 -24.170	20.361	1.00	0.00	3A7
ATOM	2063	CB .	ILE	300	33.32	1 -23.832	19.229	1.00	0.00	3A7
ATOM	2064	CG2	ILE	300	32.84	3 -22.603	18.412	1.00	0.00	3A7
MOTA	2065	CG1	ILE	300		2 -23.560	19.774	1.00	0.00	3A7
MOTA	2066	CD	ILE	300		1 -23.539	18.691	1.00	0.00	3A7
atom	2067	С	ILE	300		7 -24.293	19.764	1.00	0.00	3A7
MOTA	2068	0	ILE	300		2 -23.398	19.914	1.00	0.00	3A7
ATOM	2069	N	ILE	301		5 -25.431	19.092	1.00	0.00	3A7
ATOM	2070	CA	ILE	301		8 -25.676 5 -26.900	18.455 17.553	1.00	0.00	3A7 3A7
ATOM	2071 2072	CB	ile ile	301 301		2 -27.772	17.525	1.00	0.00	3A7
ATOM ATOM	2072		ILE	301		4 -26.460	16.091	1.00	0.00	3A7
ATOM	2074	CD	ILE	301		3 -25.647	15.869	1.00	0.00	3A7
ATOM	2075	c	ILE	301		3 -25.792	19.465	1.00	0.00	3A7
ATOM	2076	ō	ILE	301		2 -25.379	19.205	1.00	0.00	3A7
ATOM	2077	N	PHE	302	28.58	4 -26.318	20.673	1.00	0.00	3A7
ATOM	2078	CA	PHE	302	27.59	3 -26.507	21.709	1.00	0.00	3A7
MOTA	2079	CB	PHE	302		2 -27.306	22.878	1.00	0.00	3A7
ATOM .	2080	CG	PHE	302		9 -28.790	22.660	1.00	0.00	3A7
ATOM	2081		PHE	302		8 -29.335	21.379	1.00	0.00	3A7
ATOM	2082		PHE	302		0 -29.577	23.757	1.00	0.00	3A7
MOTA	2083		PHE	302		4 -30.584	21.188	1.00	0.00	3A7
ATOM	2084	CE2	PHE PHE	302 302		0 -30.829 6 -31.311	23.567 22.282	1.00	0.00	3A7 3A7
ATOM ATOM	2085 2086	C	PHE	302		1 -25.150	22.252	1.00	0.00	3A7
ATOM	2087	o	PHE	302		0 -24.892	22.478	1.00	0.00	3A7
ATOM	2088	N	ILE	303		4 -24.221	22.452	1.00	0.00	3A7
ATOM	2089	CA	ILE	303		6 -22.889	22.966	1.00	0.00	3A7
ATOM	2090	СВ	ILE	303	29.09	1 -22.188	23.539	1.00	0.00	3A7
ATOM	2091	CG2	ILE	303	28.71	6 -20.768	24.038	1.00	0.00	3A7
MOTA	2092	CG1	ILE	303	29.64	2 -23.043	24.700	1.00	0.00	3A7
MOTA	2093	CD	ILE	303		2 -22.513	25.280	1.00	0.00	3A7
MOTA	2094	С	ILE	303		5 -22.030	21.914	1.00	0.00	3A7
ATOM	2095	0	ILE	303		7 -21.376	22.173	1.00	0.00	3A7
ATOM	2096	N	PHE	304		8 -22.042	20.671	1.00	0.00	3A7 3A7
ATOM ATOM	2097 2098	CA CB	PHE	304 304		7 -21.301 7 -21.579	19.548 18.314	1.00	0.00	3A7
ATOM	2099	CG	PHE	304		9 -20.996	16.996	1.00	0.00	3A7
ATOM	2100		PHE	304		9 -19.644	16.704	1.00	0.00	3A7
ATOM	2101		PHE	304		1 -21.829	16.036	1.00	0.00	3A7
ATOM	2102		PHE	304		6 -19.134	15.472	1.00	0.00	3A7
ATOM	2103		PHE	304		8 -21.320	14.811	1.00	0.00	3A7
ATOM	2104	CZ	PHE	304		1 -19.970	14.526	1.00	0.00	3A7
ATOM	2105	С	PHE	304		2 -21.649	19.207	1.00	0.00	3A7
ATOM	2106	0	PHE	304		9 -20.780	19.129	1.00	0.00	3A7
ATOM	2107	N	ALA	305		3 -22.954	19.027	1.00	0.00	3A7
MOTA	2108	CA	ALA	305		3 -23.428	18.672	1.00	0.00	3A7
ATOM	2109	СВ	ALA	305		6 -24.883	18.216	1.00	0.00	3A7
ATOM	2110		ALA	305		4 -23.354	19.820	1.00	0.00	3A7
ATOM	2111	0	ALA	305		1 -23.132	19.620	1.00	0.00	3A7
ATOM	2112	N	GLY	306 306		4 -23.533 3 -23.642	21.051 22.219	1.00	0.00	3A7 3A7
ATOM ATOM	2113 2114	CA C	GLY GLY	306 306		3 -23.642 1 -22.346	22.219	1.00	0.00	3A7
MOTA	2115	ò	GLY	306		B -22.258	23.561	1.00	0.00	3A7
ATOM	2116	N	TYR	307		9 -21.285	22.742	1.00	0.00	

ATOM	2117	CA	TYR	307	23.134 -20.0	54 23.474	1.00	0.00	3A7
ATOM	2118	СВ	TYR	30 <b>7</b>	24.473 -19.2		1.00	0.00	3A7
ATOM	2119	CG	TYR	307	24.492 -17.7		1.00	0.00	3A7
MOTA	2120		TYR	307	23.675 -16.9		1.00	0.00	3A7 3A7
ATOM	2121 2122		TYR TYR	307 307	25.364 -17.1 23.720 -15.5		1.00	0.00	3A7
ATOM ATOM	2123		TYR	307	25.420 -15.8		1.00	0.00	3A7
ATOM	2124	cz	TYR	307	24.595 -14.9		1.00	0.00	3A7
ATOM	2125	ОН	TYR	307	24.653 -13.5		1.00	0.00	3A7
ATOM	2126	С	TYR	307	22.056 -19.2		1.00	0.00	3A7
MOTA	2127	0	TYR	307	21.092 -18.8		1.00	0.00	3A7 3A7
ATOM	2128	N	GLU	308	22.222 -18.8 21.442 -17.8		1.00	0.00	3A7
ATOM ATOM	2129 2130	CA CB	GLU	308 308	22.048 -17.5		1.00	0.00	3A7
ATOM	2131	CG	GLU	308	22.280 -18.8		1.00	0.00	3A7
ATOM	2132	CD	GLU	308	23.057 -18.5		1.00	0.00	3A7
ATOM	2133		GLU	308	23.277 -17.3		1.00	0.00	3A7
ATOM	2134		GLU	308	23.430 -19.5		1.00	0.00 0.00	3A7 3A7
ATOM ATOM	2135 2136	С 0	GLU GLU	308 308	20.007 -18.2 19.119 -17.4		1.00	0.00	3A7
ATOM	2137	N	THR	309	19.741 -19.5		1.00	0.00	3A7
ATOM	2138	CA	THR	309	18.413 -20.0		1.00	0.00	3 <b>A</b> 7
ATOM	2139	СВ	THR	309	18.504 -21.4		1.00	0.00	3A7
ATOM	2140		THR	309	17.244 -21.8		1.00	0.00	3A7 3A7
ATOM	2141		THR	309	19.256 -22.4 17.592 -20.0		1.00	0.00 0.00	3A7 3A7
ATOM ATOM	2142 2143	С 0	THR	309 309	16.436 -19.6		1.00	0.00	3A7
ATOM	2144	N	THR	310	18.187 -20.5		1.00	0.00	3A7
ATOM	2145	CA	THR	310	17.519 -20.5		1.00	0.00	3A7
ATOM	2146	CB	THR	310	18.271 -21.4		1.00	0.00	3A7
ATOM	2147		THR	310	18.739 -22.6		1.00	0.00	3A7 3A7
ATOM	2148 2149	CGZ	THR	310 310	17.383 -21.8 17.233 -19.2		1.00	0.00	3A7
ATOM ATOM	2150	Ö	THR	310	16.168 -18.9		1.00	0.00	3A7
ATOM	2151	N	SER	311	18.147 -18.2		1.00	0.00	3A7
MOTA	2152	·CA	SER	311	17.925 -16.8		1.00	0.00	3A7
ATOM	2153	CB	SER	311	19.171 -15.9		1.00	0.00	3A7 3A7
ATOM	2154	OG C	SER SER	311 311	20.346 -16.7 16.857 -16.1		1.00	0.00	3A7
ATOM ATOM	2155 2156	с 0	SER	311	15.998 -15.5		1.00	0.00	3A7
ATOM	2157	N	SER	312	16.848 -16.3		1.00	0.00	3A7
ATOM	2158	CA	SER	312	15.858 -15.7		1.00	0.00	3A7
ATOM	2159	СВ	SER	312	16.203 -15.8		1.00	0.00	3A7
ATOM	2160	OG	SER	312	16.398 -17.2 14.473 -16.3		1.00	0.00	3A7 3A7
ATOM ATOM	2161 2162	С 0	SER SER	312 312	13.477 -15.0		1.00	0.00	3A7
ATOM	2163	N	VAL	313	14.376 -17.6		1.00	0.00	3A7
ATOM	2164	CA	VAL	313	13.115 -18.2	232 22.678	1.00	0.00	3A7
MOTA	2165	ÇΒ	VAL	313	13.262 -19.7		1.00	0.00	3A7
MOTA	2166		VAL	313	12.003 -20.4 13.426 -20.3		1.00	0.00	3A7 3A7
MOTA MOTA	2167 2168	CG2	VAL VAL	313 313	12.555 -17.		1.00	0.00	3A7
ATOM	2169	ŏ	VAL	313	11.368 -17.4		1.00	0.00	3A7
MOTA	2170	N	LEU	314	13.406 -17.5	25.000	1.00	0.00	3A7
ATOM	2171	CA	LEU	314	13.003 -16.9		1.00	0.00	3A7
MOTA	2172	CB	LEU	314	14.178 -17.0		1.00	0.00	3A7 3A7
ATOM	2173 2174	CG	LEU LEU	314 314	14.712 -18.4 16.160 -18.4		1.00	0.00	3A7
ATOM ATOM	2175		LEU	314	13.817 -19.3		1.00	0.00	3A7
ATOM	2176	c	LEU	314	12.519 -15.		1.00	0.00	3A7
ATOM	2177	0	LEU	314	11.490 -15.3		1.00	0.00	3A7
MOTA	2178	N	SER	315	13.252 -14.		1.00	0.00	3A7
ATOM	2179 2180	CA	SER	315 315	12.914 -13.3 14.033 -12.0		1.00	0.00	3A7 3A7
ATOM ATOM	2180	ĊВ OG	SER SER	315	15.234 -12.0		1.00	0.00	3A7
ATOM	2182	c	SER	315	11.625 -13.		1.00	0.00	3A7
MOTA	2183	0	SER	315	10.814 -12.		1.00	0.00	3A7
ATOM	2184	N	PHE	316	11.391 -14.0		1.00	0.00	3A7
ATOM	2185	CA	PHE	316	10.164 -14.6 10.264 -14.5		1.00	0.00	3A7 3A7
ATOM ATOM	2186 2187	CB CG	PHE	316 316	10.697 -14.6		1.00	0.00	3A7
ATOM	2188		PHE	316	11.810 -14.		1.00	0.00	3A7

ATOM	2189	CD2	PHE	316	9.933	-12.985	19.709	1.00	0.00	3A7
ATOM	2190	CEI		316		-13.699	18.217	1.00	0.00	3A7
ATOM	2191	CE2		316		-12.246	18.582	1.00	0.00	3A7
ATOM	2192	CZ	PHE	316	11.402	-12.600	17.837	1.00	0.00	3A7
MOTA	2193	С	PHE	316	9.015	-14.618	23.406	1.00	0.00	3A7
ATOM	2194	0	PHE	316	7.891	-14.133	23.296	1.00	0.00	3A7
MOTA	2195	N	ILE	317	9.257	-15.617	24.306	1.00	0.00	3A7
MOTA	2196	CA	ILE	317		-16.171	25.144	1.00	0.00	3A7
ATOM	2197	СВ	ILE	317		-17.418	26.022	1.00	0.00	3A7
ATOM	2198	CG2	ILE	317	7.716	-17.454	27.357	1.00	0.00	3A7
MOTA	2199	CG1	ILE	317		-18.749	25.331	1.00	0.00	3A7
MOTA	2200	CD	ILE	317		-19.340	24.419	1.00	0.00	3A7
MOTA	2201	С	ILE	317		-15.117	26.091	1.00	0.00	3A7
MOTA	2202	0	ILE	317		-14.997	26.274	1.00	0.00	3A7
ATOM	2203	N	ILE	318		-14.313	26.715	1.00	0.00	3A7
ATOM	2204	CA	ILE	318		-13.252	27.635	1.00	0.00	3A7
ATOM	2205	CB	ILE	318		-12.624	28.274	1.00	0.00	3A7 3A7
MOTA	2206	CG2		318		-11.357	29.092	1.00	0.00	
MOTA	2207	CG1		318		-13.689	29.181	1.00	0.00	3A7 3A7
ATOM	2208	CD	ILE	318		-13.295	29.665	1.00	0.00	3A7
ATOM	2209	C	ILE	318		-12.213	26.942	1.00	0.00	3A7
MOTA	2210	0	ILE	318		-11.802	27.441 25.716	1.00	0.00	3A7
MOTA	2211	N	TYR	319		-11.823	24.906	1.00	0.00	3A7
ATOM	2212	CA	TYR	319		-10.893 -10.658	23.571	1.00	0.00	3A7
ATOM	2213	CB	TYR	319 319	6.940		22.557	1.00	0.00	3A7
ATOM	2214	CG	TYR TYR		6.414	-8.628	22.863	1.00	0.00	3A7
MOTA	2215 2216	CD2		319 319		-10.438	21.301	1.00	0.00	3A7
ATOM ATOM	2217		TYR	319	5.597	-7.976	21.949	1.00	0.00	3A7
MOTA	2218		TYR	319	5.898		20.375	1.00	0.00	3 <b>A</b> 7
ATOM	2219	CZ	TYR	319	5.336		20.704	1.00	0.00	3A7
ATOM	2220	ОН	TYR	319	4.491	-7.887	19.783	1.00	0.00	3A7
ATOM	2221	C	TYR	319		-11.359	24.631	1.00	0.00	3A7
ATOM	2222	ŏ	TYR	319		-10.588	24.752	1.00	0.00	3A7
ATOM	2223	N	GLU	320		-12.651	24.277	1.00	0.00	3A7
ATOM	2224	CA	GLU	320		-13.205	23.952	1.00	0.00	3A7
ATOM	2225	CB	GLU	320	4.190	-14.545	23.220	1.00	0.00	3A7
ATOM	2226	CG	GLU	320	4.824	-14.416	21.829	1.00	0.00	3A7
ATOM	2227	CD	GLU	320	3.795	-13.768	20.915	1.00	0.00	3A7
ATOM	2228	OE1	GLU	320	4.068	-12.634	20.435	1.00	0.00	3A7
MOTA	2229	OE2	GLU	320	2.723	-14.384	20.681	1.00	0.00	3A7
ATOM	2230	С	GĻŲ	320	3.209	-13.345	25.140	1.00	0.00	3A7
ATOM	2231	0	GLU	320		-13.087	25.041	1.00	0.00	3A7
ATOM	2232	N	LEU	321		-13.705	26.321	1.00	0.00	3A7
ATOM	2233	CA	LEU	321		-13.799	27.537	1.00	0.00	3A7
ATOM	2234	СВ	LEU	321		-14.427	28.662	1.00	0.00	3A7
MOTA	2235	CG	LEU	321		-15.941	28.472	1.00	0.00	3A7 3A7
ATOM	2236		LEU	321		-16.456	29.453	1.00	0.00	3A7
ATOM	.2237		LEU	321		-16.706	28.641	1.00	0.0Q 0.00	3A7
ATOM	2238	C	LEU	321		-12.447	28.007 28.509	1.00	0.00	3A7
ATOM	2239	0	LEU	321		-12.302 -11.421	27.837	1.00	0.00	3A7
ATOM	2240	N	ALA	322 322		-10.068	28.220	1.00	0.00	3A7
ATOM	2241	CA CB	ALA ALA	322		-9.229				3A7
ATOM	2242 2243	C	ALA	322	2.044		27.279	1.00	0.00	3A7
ATOM ATOM	2244	Ö	ALA	322	1.166		27.668	1.00	0.00	3A7
ATOM	2245	N	THR	323	2.110		25.996	1.00	0.00	3A7
ATOM	2246	CA	THR	323	1.174		25.006	1.00	0.00	3A7
ATOM	2247	CB	THR	323	1.714		23.612	1.00	0.00	3A7
ATOM	2248		THR	323		-10.786	23.282	1.00	0.00	3A7
ATOM	2249		THR	323	2.782		23.418	1.00	0.00	3A7
ATOM	2250	c	THR	323	-0.164	-10.105	25.063	1.00	0.00	3A7
ATOM	2251	ō	THR	323	-1.132		24.486	1.00	0.00	3A7
ATOM	2252	N	HIS	324		-11.241	25.774	1.00	0.00	3A7
ATOM	2253	CA	HIS	324		-12.018	25.882	1.00	0.00	3A7
ATOM	2254		HIS	324	-2.250	-12.554	22.767	1.00	0.00	3A7
ATOM	2255	CG	HIS	324	-1.279	-13.139	23.576	1.00	0.00	3A7
MOTA	2256	СВ	HIS	324		-13.311	25.087	1.00	0.00	3A7
MOTA	2257		HIS	324		-12.447	21.617	1.00	0.00	3A7
MOTA	2258		HIS	324		-13.016	22.856	1.00		3A7
MOTA	2259	CE1	HIS	324		-12.187	21.610	1.00	0.00	3A7
ATOM	2260	C	HIS	324	-1.699	-12.327	27.334	1.00	0.00	3A7

ATOM	2261	0	HIS	324	-1.410	-13.448	27.764	1.00	0.00	3A7
ATOM	2262	N	PRO	325		-11.398	28.139	1.00	0.00	3A7
ATOM	2263	CA	PRO	325		-11.530	29.587	1.00	0.00	3A7
		CD	PRO	325		-10.073	27.697	1.00	0.00	3A7
ATOM	2264					-10.217	30.049	1.00	0.00	3A7
ATOM	2265	CB	PRO	325			28.959	1.00	0.00	3A7
ATOM	2266	CG	PRO	325	-2.634	-9.212				3A7
ATOM	2267	С	PRO	325		-12.703	30.001	1.00	0.00	
ATOM	2268	0	PRO	325		-13.255	31.072	1.00	0.00	3A7
MOTA	2269	N	ASP	326		-13.144	29.162	1.00	0.00	3A7
ATOM	2270	CA	ASP	326	-5.016	-14.290	29.448	1.00	0.00	3A7
ATOM	2271	СВ	ASP	326	-6.108	-14.480	28.372	1.00	0.00	3A7
MOTA	2272	CG	ASP	326	-7.091	-13.305	28.363	1.00	0.00	3A7
ATOM	2273	OD1	ASP	326	-7.016	-12.435	29.271	1.00	0.00	3A7
ATOM	2274		ASP	326		-13.276	27.437	1.00	0.00	3A7
ATOM	2275	c	ASP	326		-15.557	29.518	1.00	0.00	3A7
ATOM	2276	ŏ	ASP	326		-16.408	30.379	1.00	0.00	3A7
				327		-15.680	28.617	1.00	0.00	3A7
ATOM	2277	N	VAL				28.551	1.00	0.00	3A7
MOTA	2278	CA	VAL	327		-16.822				3A7
ATOM	2279	СВ	VAL	327		-16.855	27.249	1.00	0.00	
ATOM	2280		VAL	327		-18.114	27.189	1.00	0.00	3A7
ATOM	2281	CG2	VAL	327		-16.830	26.078	1.00	0.00	3A7
ATOM	2282	С	VAL	327	-1.357	-16.811	29.718	1.00	0.00	3A7
ATOM	2283	0	VAL	327	-1.126	-17.833	30.353	1.00	0.00	3A7
MOTA	2284	N	GLN	328	-0.822	-15.622	30.057	1.00	0.00	3A7
ATOM	2285	CA	GLN	328	0.054	-15.440	31.190	1.00	0.00	3A7
ATOM	2286	CB	GLN	328		-13.994	31.280	1.00	0.00	3A7
ATOM	2287	CG	GLN	328		-13.874	31.956	1.00	0.00	3A7
	2288	CD	GLN	328		-12.432	31.850	1.00	0.00	3A7
ATOM				328		-11.512	31.507	1.00	0.00	3A7
ATOM	2289		GLN			-12.247	32.162	1.00	0.00	3A7
ATOM	2290		GLN	328					0.00	3A7
MOTA	2291	С	GLN	328		-15.809	32.500	1.00		
ATOM	2292	0	GLN	328		-16.448	33.339	1.00	0.00	3A7
MOTA	2293	N	GLN	329		-15.438	32.692	1.00	0.00	3A7
MOTA	2294	CA	GLN	329	-2.599	-15.749	33.879	1.00	0.00	3A7
ATOM	2295	CB	GLN	329	-3.961	-15.032	33.870	1.00	0.00	3A7
MOTA	2296	CG	GLN	329	-3.832	-13.525	34.148	1.00	0.00	3A7
ATOM	2297	CD	GLN	329	-5.215	-12.882	34.023	1.00	0.00	3A7 -
ATOM	2298	OE1	GLN	329	-6.121	-13.175	34.813	1.00	0.00	3A7
ATOM	2299		GLN	329		-11.987	33.000	1.00	0.00	3A7
ATOM	2300	C	GLN	329		-17.226	34.022	1.00	0.00	3A7
ATOM	2301	ō	GLN	329		-17.780	35.102	1.00	0.00	3A7
ATOM	2302	N	LYS	330		-17.913	32.907	1.00	0.00	3A7
ATOM	2303	CA	LYS	330		-19.343	32.883	1.00	0.00	3A7
ATOM	2304	СВ	LYS	330		-19.754	31.503	1.00	0.00	3A7
						-21.169	31.446	1.00	0.00	3A7
ATOM	2305	CG	LYS	330			30.124	1.00	0.00	3A7
ATOM	2306	CD	LYS	330		-21.428		1.00		3A7
MOTA	2307	CE	LYS	330		-22.799	30.054		0.00	3A7
MOTA	2308	NZ	LYS	330		-22.943	31.113	1.00	0.00	
. ATOM	2309	С	LYS	330	•	-20.090	33.241	1.00	0.00	3A7
ATOM	2310	0	LYS	330		-21.027	34.040	1.00	0.00	3A7
ATOM	2311	N	VAL	331		-19.618	32.704	1.00	0.00	3A7
ATOM	2312	CA	VAL	331		-20.189	32.957	1.00	0.00	3A7
ATOM	2313	СВ	VAL	331		-19.605	32.030	1.00	0.00	3A7
MOTA	2314	CG1	VAL	331	2.843	-20.076	32.382	1.00	0.00	3A7
ATOM	2315	CG2	VAL	331	1.080	-20.072	30.601	1.00	0.00	3A7
ATOM	2316	C	VAL	331		-19.992	34.390	1.00	0.00	3A7
ATOM	2317	ŏ	VAL	331		-20.919	35.023	1.00	0.00	3A7
ATOM	2318	N	GLN	332		-18.783	34.951	1.00	0.00	3A7
ATOM	2319	CA	GLN	332		-18.455	36.319	1.00	0.00	3A7
						-16.968	36.628	1.00	0.00	3A7
ATOM	2320	CB	GLN	332		-16.072	36.011	1.00	0.00	3A7
ATOM	2321	CG	GLN	332			36.311	1.00	0.00	3A7
ATOM	2322	CD	GLN	332		-14.601				3A7
ATOM	2323		GLN	332		-13.947	37.057	1.00	0.00	
ATOM	2324		GLN	332		-14.079	35.701	1.00	0.00	3A7
ATOM	2325	С	GLN	332		-19.234	37.311	1.00	0.00	3A7
ATOM	2326	0	GLN	332		-19.634	38.351	1.00	0.00	3A7
ATOM	2327	N	LYS	333		-19.512	36.991	1.00	0.00	3A7
ATOM	232B	CA	LYS	333	-2.087	-20.320	37.797	1.00	0.00	3 <b>A</b> 7
ATOM	2329	СВ	LYS	333	-3.508	-20.312	37.204	1.00	0.00	3A7
ATOM	2330	CG	LYS	333	-4.571	-21.052	38.035	1.00	0.00	3A7
ATOM	2331	CD	LYS	333		-20.945	37.441	1.00	0.00	3A7
ATOM	2332	CE	LYS	333		-21.617	36.068	1.00	0.00	3A7
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ATOM	2333	NZ	LYS	333	-7.518	-21.516	35.576	1.00	0.00	3A7
ATOM	2334	c	LYS	333		-21.746	37.882	1.00	0.00	3A7
				333		-22.344	38.954	1.00	0.00	3A7
MOTA	2335	0	LYS							3A7
ATOM	2336	N	GLU	334		-22.295	36.728	1.00	0.00	
ATOM	2337	CA	GLU	334		-23.579	36.649	1.00	0.00	3A7
ATOM	2338	CB	GLU	334	-0.149	-23.952	35.224	1.00	0.00	3A7
MOTA	2339	CG	GLU	334	-0.038	-25.481	35.122	1.00	0.00	3A7
ATOM	2340	CD	GLU	334	0.087	-25.922	33.672	1.00	0.00	3A7
ATOM	2341		GLU	334		-26.779	33.251	1.00	0.00	3A7
						-25.424	32.971	1.00	0.00	3A7
ATOM	2342		GLU	334					0.00	3A7
MOTA	2343	С	GLU	334		-23.722	37.472	1.00		
ATOM	2344	0	GLU	334		-24.667	38.236	1.00	0.00	3A7
MOTA	2345	N	ILE	335	1.627	-22.744	37.370	1.00	0.00	3A7
ATOM	2346	CA	ILE	335	2.874	-22.692	38.098	1.00	0.00	3A7
MOTA	2347	СВ	ILE	335	3.672	-21.474	37.679	1.00	0.00	3A7
ATOM	2348		ILE	335		-21.230	38.599	1.00	0.00	3A7
ATOM			ILE	335		-21.660	36.215	1.00	0.00	3A7
	2349							1.00	0.00	3A7
MOTA	2350	CD	ILE	335		-20.360	35.597			
ATOM	2351	С	ILE	335		-22.684	39.587	1.00	0.00	3A7
ATOM	2352	0	ILE	335	3.219	-23.480	40.320	1.00	0.00	3A7
ATOM	2353	N	ASP	336	1.727	-21.822	40.071	1.00	0.00	3A7
ATOM	2354	CA	ASP	336	1.416	-21.706	41.476	1.00	0.00	3A7
ATOM	2355	CB	ASP	336		-20.565	41.750	1.00	0.00	3A7
	2356	CG	ASP	336		-19.199	41.420	1.00	0.00	3A7
MOTA						-19.127	41.123	1.00	0.00	3A7
MOTA	2357		ASP	336					0.00	3A7
ATOM	2358		ASP	336		-18.199	41.470	1.00		
MOTA	2359	С	ASP	336		-22.996	42.010	1.00	0.00	3A7
ATOM	2360	0	ASP	336	1.183	-23.420	43.106	1.00	0.00	3A7
MOTA	2361	N	THR	337	-0.022	-23.674	41.213	1.00	0.00	3A7
ATOM	2362	CA	THR	337	-0.701	-24.903	41.571	1.00	0.00	3A7
ATOM	2363	СВ	THR	337		-25.156	40.609	1.00	0.00	3A7
	2364		THR	337		-24.092	40.721	1.00	0.00	3A7
MOTA						-26.473	40.896	1.00	0.00	3A7
ATOM	2365		THR	337						3A7
MOTA	2366	С	THR	337		-26.114	41.595	1.00	0.00	
MOTA	2367	0	THR	337		-27.000	42.433	1.00	0.00	3A7
MOTA	2368	N	VAL	338	1.202	-26.189	40.667	1.00	0.00	3A7
MOTA	2369	CA	VAL	338	2.055	-27.349	40.503	1.00	0.00	3A7
MOTA	2370	CB	VAL	338	2.466	-27.564	39.051	1.00	0.00	7א3
ATOM	2371		VAL	338	3.403	-28.783	38.900	1.00	0.00	3A7
ATOM	2372		VAL	338		-27.789	38.226	1.00	0.00	3A7
				338		-27.232	41.404	1.00	0.00	3A7
MOTA	2373	С	VAL				42.113		0.00	3A7
MOTA	2374	0	VAL	338		-28.178		1.00		
MOTA	2375	N	LEU	339		-26.065	41.421	1.00	0.00	3A7
ATOM	2376	CA	LEU	339	5.053	-25.835	42.331	1.00	0.00	3A7
MOTA	2377	CB	LEU	339	6.213	-25.014	41.736	1.00	0.00	3A7
ATOM	2378	CG	LEU	339	7.082	-25.819	40.766	1.00	0.00	. 3A7
ATOM	2379		LEU	339	8.159	-24.904	40.176	1.00	0.00	3A7
ATOM	2380		LEU	339		-27.051	41.439	1.00	0.00	3A7
ATOM	2381		LEU	339		-25.038	43.521	1.00	0.00	3A7
		C							0.00	3A7
ATOM	2382	0	LEU	339		-23.878	43.325	1.00		
ATOM	23 <b>83</b>	N	PRO	340		-25.565	44.752	1.00	0.00	3A7
MOTA	2384	CA	PRO	340		-24.851	45.907	1.00	0.00	3A7
ATOM	2385	CD	PRO	340	4.660	-26.986	45.025	1.00	0.00	3A7
ATOM	2386	CB	PRO	340	3.483	-25.968	46.840	1.00	0.00	3A7
ATOM	2387	CG	PRO	340	4.398	-27.154	46.523	1.00	0.00	3A7
ATOM	2388	С	PRO	340		-24.042	46.550	1.00	0.00	3A7
ATOM	2389	ŏ	PRO	340		-24.463	46.512	1.00	0.00	3A7
ATOM				341		-22.893	47.182	1.00	0.00	3A7
	2390	N	ASN					1.00	0.00	3A7
ATOM	2391	CA	ASN	341		-22.073	48.065			
ATOM	2392	СВ	ASN	341		-22.872	49.244	1.00	0.00	3A7
ATOM	2393	CG	ASN	341		-23.614	50.023	1.00	0.00	3A7
ATOM	2394	OD1	ASN	341	5.051	-24.850	50.059	1.00	0.00	3A7
ATOM	2395		ASN	341	4.155	-22.826	50.663	1.00	0.00	3A7
ATOM	2396	c	ASN	341		-21.330	47.312	1.00	0.00	3A7
ATOM	2397	ŏ	ASN	341		-20.897	-46.178	1.00	0.00	3A7
						-21.175	47.953	1.00	0.00	3A7
ATOM	2398	N	LYS	342						3A7
ATOM	2399	CA	LYS	342		-20.529	47.396	1.00	0.00	
ATOM	2400	СВ	LYS	342		-19.456	48.339	1.00	0.00	
MOTA	2401	CG	LYS	342		-18.309	48.647	1.00	0.00	3A7
ATOM	2402	CD	LYS	342	9.210	-17.205	49.527	1.00	0.00	3A7
ATOM	2403	CE	LYS	342	9.570	-17.674	50.944	1.00	0.00	3A7
ATOM	2404	NZ	LYS	342		-16.560	51.741	1.00	0.00	3A7
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ATOM	2405	С	LYS	342	10.016	-21.594	47.146	1.00	0.00	3A7
ATOM	2406	0	LYS	342		-21.442	47.515	1.00	0.00	3A7
ATOM	2407	'N	ALA	343	9.595	-22.711	46.501	1.00	0.00	3A7
ATOM	2408	CA	ALA	343	10.434	-23.839	46.171	1.00	0.00	3A7
ATOM	2409	CB	ALA	343	9.750		46.468	1.00	0.00	3A7
ATOM	2410	С	ALA	343		-23.763	44.700	1.00	0.00	3A7
MOTA	2411	0	ALA	343		-23.520	43.911	1.00	0.00	3A7
ATOM	2412	N	PRO	344		-24.000	44.274	1.00	0.00	3A7
ATOM	2413	CA	PRO	344		-24.110	42.875	1.00	0.00	3A7 3A7
MOTA	2414	CD	PRO	344		-23.771 -24.072	45.118 42.880	1.00	0.00	3A7
ATOM	2415 2416	CB CG	PRO PRO	344 344		-23.318	44.160	1.00	0.00	3A7
ATOM ATOM	2417	C	PRO	344		-25.414	42.274	1.00	0.00	3A7
MOTA	2418	ŏ	PRO	344		-26.289	43.033	1.00	0.00	3A7
ATOM	2419	N	PRO	345		-25.589	40.953	1.00	0.00	3A7
MOTA	2420	CA	PRO	345		-26.737	40.270	1.00	0.00	3A7
ATOM	2421	CD	PRO	345	12.098	-24.479	40.043	1.00	0.00	3A7
MOTA	2422	CB	PRO	345	11.402	-26.382	38.778	1.00	0.00	3A7
MOTA	2423	CG	PRO	345		-24.857	38.731	1.00	0.00	3A7
ATOM	2424	С	PRO	345		-27.996	40.521	1.00	0.00	3A7
ATOM	2425	0	PRO	345		-27.934	40.723	1.00	0.00	3A7
MOTA	2426	N	THR	346		-29.156	40.428	1.00	0.00	3A7 3A7
ATOM	2427	CA	THR	346		-30.434	40.286 41.180	1.00	0.00	3A7
ATOM	2428	CB	THR	346		-31.522 -31.633	41.100	1.00	0.00	3A7
ATOM	2429 2430		THR	346 346		-31.183	42.644	1.00	0.00	3A7
ATOM ATOM	2430	C	THR	346		-30.751	38.827	1.00	0.00	3A7
ATOM	2432	ō	THR	346		-29.983	38.054	1.00	0.00	3A7
ATOM	2433	N	TYR	347		-31.922	38.405	1.00	0.00	3A7
ATOM	2434	CA	TYR	347		-32.298	37.022	1.00	0.00	3A7
ATOM	2435	СВ	TYR	347	13.345	-33.383	36.599	1.00	0.00	3A7
MOTA	2436	CG	TYR	347		-34.221	37.758	1.00	0.00	3A7
MOTA	2437	CD1	TYR	347		-35.455	38.007	1.00	0.00	3A7
MOTA	2438		TYR	347		-33.809	38.584	1.00	0.00	3A7
ATOM	2439		TYR	347		-36.258	39.060	1.00	0.00	3A7
ATOM	2440		TYR	347		-34.609	39.638	1.00	0.00	3A7 3A7
ATOM	2441	CZ	TYR	347		-35.835	39.877	1.00	0.00	3A7
ATOM	2442	ОН	TYR	347 347		-36.649 -32.842	40.945 36.741	1.00	0.00	3A7
ATOM ATOM	2443 2444	С О	TYR TYR	347		-32.653	35.655	1.00	0.00	3A7
ATOM	2445	N	ASP	348		-33.487	37.746	1.00	0.00	3A7
ATOM	2446	CA	ASP	348		-34.072	37.677	1.00	0.00	. 3A7
ATOM	2447	СВ	ASP		. 8.708	-34.785	38.996	1.00	0.00	3A7
ATOM	2448	CG	ASP	348	9.678	-35.950	39.163	1.00	0.00	3A7
ATOM	2449	OD1	ASP	348	9.665	-36.846	38.277	1.00	0.00	3A7
ATOM	2450	OD2	ASP	348		-35.959	40.167	1.00	0.00	3A7
MOTA	2451	С	ASP	348		-33.064	37.424	1.00	0.00	3A7
ATOM	2452	0	ASP	348		-33.393	36.890	1.00	0.00	3A7
MOTA	2453	N.	THR	349		-31.784	37.764	1.00	0.00	. 3A7 3A7
ATOM	2454	CA	THR	349		-30.615 -29.394	37.512 38.153	1.00	0.00	3A7
ATOM ATOM	2455 2456	CB	THR	349 349		-29.682	39.512	1.00	0.00	3A7
ATOM	2457		THR	349		-28.168	38.103	1.00	0.00	3A7
ATOM	2458	C	THR	349		-30.355	36.030	1.00	0.00	3A7
ATOM	2459	ŏ	THR	349		-29.855	35.582	1.00	0.00	3A7
MOTA	2460	N	VAL	350		-30.735	35.203	1.00	0.00	3A7
ATOM	2461	CA	VAL	350	8.261	-30.585	33.760	1.00	0.00	3A7
MOTA	2462	CB	VAL	350		-31.111	33.245	1.00	0.00	3A7
ATOM	2463		VAL	350		-31.257	31.710	1.00	0.00	3A7
ATOM	2464		VAL	350		-30.188	33.784	1.00	0.00	3A7
ATOM	2465	C	VAL	350		-31.305	33.054	1.00	0.00	3A7
ATOM	2466	0	VAL	350		-30.900	31.980	1.00	0.00	3A7 3A7
ATOM	2467	N	LEU	351		-32.397	33.667	1.00	0.00	3A7
ATOM	2468	CA	LEU	351 351		-33.220 -34.682	33.098 33.599	1.00	0.00	3A7
ATOM ATOM	2469 2470	CB CG	LEU	351 351		-34.662	33.359	1.00	0.00	3A7
ATOM	2471		LEU	351		-36.712	34.024	1.00	0.00	3A7
ATOM	2472		LEU	351		-35.402	31.865	1.00	0.00	3A7
ATOM	2473	c	LEU	351		-32.710	33.432	1.00	0.00	3A7
ATOM	2474	ŏ	LEU	351		-32.996	32.716	1.00	0.00	3A7
ATOM	2475	N	GLN	352		-31.949	34.546	1.00	0.00	3A7
ATOM	2476	CA	GLN	352	2.775	-31.491	35.037	1.00	0.00	3A7

ATOM	2477	СВ	GLN	352	2.625	-31.677	36.565	1.00	0.00	3A7
ATOM	2478	CG	GLN	352	2.109	-33.072	36.977	1.00	0.00	3A7
MOTA	2479	CD	GLN	352	3.125	-34.176	36.678	1.00	0.00	3A7
ATOM	2480	0El	GLN	352	2.971	-34.938	35.716	1.00	0.00	3A7
MOTA	2481	NE2	GLN	352	4.173	-34.268	37.551	1.00	0.00	3A7
ATOM	2482	С	GLN	352	2.540	-30.043	34.711	1.00	0.00	3A7
MOTA	2483	0	GLN	352		-29.394	35.333	1.00	0.00	3A7
MOTA	2484	N	LEU	353	3.254	-29.494	33.712	1.00	0.00	3A7
MOTA	2485	CA	LEU	353	3.130	-28.104	33.338	1.00	0.00	3A7
ATOM	2486	CB	LEU	353		-27.396	33.371	1.00	0.00	3A7
MOTA	2487	CG	LEU	353 .		-27.076	34.789	1.00	0.00	3A7
ATOM	2488		LEU	353		-26.787	34.712	1.00	0.00	3A7
MOTA	2489	CD2	LEU	353		-25.911	35.433	1.00	0.00	3A7
MOTA	2490	С	LEU	353		-28.000	31.951	1.00	0.00	3A7
ATOM	2491	0	LEU	353		-27.396	31.071	1.00	0.00	3A7
ATOM	2492	N	GLU	354		-28.556	31.747	1.00	0.00	3A7
ATOM	2493	CA	GLU	354		-28.679	30.481	1.00	0.00	3A7
MOTA	2494	СВ	GLU	354		-29.284	30.692	1.00	0.00	3A7
ATOM	2495	CG	GLU	354		-30.790	31.013	1.00	0.00	3A7
ATOM	2496	CD	GLU	354		-31.081	32.431	1.00	0.00	3A7
ATOM	2497		GLU	354		-31.962	32.579	1.00	0.00	3A7
MOTA	2498		GLU	354		-30.446	33.382	1.00	0.00	3A7
MOTA	2499	С	GLU	354		-27.384	29.710	1.00	0.00	3A7
MOTA	2500	0	GLU	354		-27.315	28.531	1.00	0.00	3A7
ATOM	2501	N	TYR	355		-26.319	30.358	1.00	0.00	3A7
MOTA	2502	CA	TYR	355		-25.056	29.708	1.00	0.00	3A7
ATOM	2503	СВ	TYR	355		-24.126	30.584	1.00	0.00	3A7
ATOM	2504	CG	TYR	355		-24.797	30.922	1.00	0.00	3A7
MOTA	2505		TYR	355		-24.843	32.245	1.00	0.00	3A7
ATOM	2506		TYR TYR	355		-25.427	29.938 32.585	1.00	0.00	3A7 3A7
ATOM	2507			355		-25.504 -26.101		1.00	0.00	3A7 3A7
ATOM	2508		TYR	355		-26.138	30.275	1.00	0.00	3A7
MOTA MOTA	2509 2510	CZ OH	TYR TYR	355 355		-26.813	31.599 31.940	1.00	0.00	3A7
ATOM	2511	C	TYR	355		-24.314	29.358	1.00	0.00	3A7
MOTA	2512	Ö	TYR	355 355		-23.672	28.320	1.00	0.00	3A7
ATOM	2513	N	LEU	356		-24.432	30.194	1.00	0.00	3A7
ATOM	2514	CA	LEU	356		-23.853	29.929	1.00	0.00	3A7
ATOM	2515	СВ	LEU	356		-24.000	31.136	1.00	0.00	3A7
ATOM	2516	CG	LEU	356		-22.859	31.211	1.00	0.00	3A7
ATOM	2517		LEU	356		-22.429	32.674	1.00	0.00	3A7
MOTA	2518		LEU	356		-23.187	30.588	1.00	0.00	3A7
ATOM	2519	С	LEU	356		-24.430	28.735	1.00	0.00	3A7
ATOM	2520	Ō	LEU	356		-23.709	27.891	1.00	0.00	3A7
ATOM	2521	N	ASP	357		-25.778	28.619	1.00	0.00	3A7
ATOM	2522	CA	ASP	357		-26.516	27.513	1.00	0.00	- 3A7
ATOM	2523	CB	ASP	357		-28.050	27.598	1.00	0.00	3A7
ATOM	2524	CG	ASP	357	5.259	-28.771	28.597	1.00	0.00	3A7
ATOM	.2525	OD1	ASP	357	5.958	-29.726	28.159	1.00	0.00	3A7
ATOM	2526	OD2	ASP	357	5.258	-28.397	29.796	1.00	0.00	3A7
ATOM	2527	С	ASP	357	4.055	-26.136	26.182	1.00	0.00	3A7
MOTA	2528	0	ASP	357	4.748	-25.985	25.183	1.00	0.00	3A7
MOTA	2529	N	MET	358	2.719	-25.956	26.163	1.00	0.00	3A7
MOTA	2530	CA	MET	358		-25.573		1.00	0.00	3A7
MOTA	2531	CB	MET	358	0.466	-25.711	25.263	1.00	0.00	3A7
MOTA	2532	CG	MET	358	0.027	-27.178	25.430	1.00	0.00	. 3A7
ATOM	2533	SD	MET	358		-27.420	26.341	1.00	0.00	3A7
MOTA	2534	CE	MET	358		-26.461	25.262	1.00	0.00	3A7
ATOM	2535	С	MET	358		-24.149	24.601	1.00	0.00	3A7
ATOM	2536	0	MET	358		-23.825	23.421	1.00	0.00	3A7
MOTA	2537	N	VAL	359		-23.255	25.594	1.00	0.00	3A7
ATOM	2538	CA	VAL	359		-21.869	25.376	1.00	0.00	3A7
ATOM	2539	CB	VAL	359		-21.083	26.684	1.00	0.00	3A7
ATOM	2540	CG1		359		-19.776	26.626	1.00	0.00	3A7
ATOM	2541	CG2		359		-20.783	27.005	1.00	0.00	3A7
ATOM	2542	C	VAL	359		-21.791	24.701	1.00	0.00	3A7
ATOM	2543	0	VAL	359		-21.063	23.725	1.00	0.00	3A7
ATOM	2544	N	VAL	360		-22.575	25.182	1.00	0.00	3A7
ATOM	2545	CA	VAL	360		-22.600	24.616	1.00	0.00	3A7
ATOM	2546	CB	VAL	360 360		-23.421	25.479	1.00	0.00	3A7
ATOM	2547	CG1		360 360		-23.573	24.831	1.00	0.00	3A7
ATOM	2548	CG2	AWP	360	. 033	-22.713	26.844	1.00	0.00	3A7

ATOM	2549	С	VAL	360	6.520	-23.153	23.207	1.00	0.00	3A7
ATOM	2550	ō	VAL	360		-22.609	22.323	1.00	0.00	3A7
ATOM	2551	N	ASN	361		-24.208	22.949	1.00	0.00	3A7
						-24.789	21.630	1.00	0.00	3A7
MOTA	2552	CA	ASN	361				1.00	0.00	3A7
MOTA	2553	СВ	ASN	361		-26.030	21.669			3A7
ATOM	2554	CG	ASN	361		-27.219	22.258	1.00	0.00	
MOTA	2555		ASN	361		-27.329	22.121	1.00	0.00	3A7
ATOM	2556		ASN	361		-28.135	22.930	1.00	0.00	3A7
ATOM	2557	С	ASN	361		-23.808	20.655	1.00	0.00	3A7
ATOM	2558	0	ASN	361	5.410	-23.694	19.523	1.00	0.00	3 <b>A7</b>
ATOM	2559	N	GLU	362	3.925	-23.044	21.087	1.00	0.00	3 <b>A</b> 7
ATOM	2560	CA	GLU	362	3.338	-21.994	20.287	1.00	0.00	3A7
ATOM	2561	СВ	GLU	362	2.013	-21.499	20.896	1.00	0.00	3A7
ATOM	2562	CG	GLU	362	1.224	-20.515	20.011	1.00	0.00	3A7
ATOM	2563	CD	GLU	362	0.583	-21.183	18.798	1.00	0.00	3A7
ATOM	2564		GLU	362	0.987	-22.314	18.429	1.00	0.00	3 <b>A</b> 7
ATOM	2565		GLU	362	-0.309	-20.534	18.190	1.00	0.00	3A7
ATOM	2566	C	GLU	362		-20.837	20.000	1.00	0.00	3A7
ATOM	2567	ō	GLU	362		-20.266	18.913	1.00	0.00	3A7
ATOM	2568	N	THR	363		-20.478	20.946	1.00	0.00	3A7
ATOM	2569	CA	THR	363		-19.416	20.720	1.00	0.00	3A7
ATOM	2570	СВ	THR	363		-19.002	21.991	1.00	0.00	3A7
ATOM	2571		THR	363		-18.623	22.938	1.00	0.00	3A7
		CG2		363		-17.778	21.706	1.00	0.00	3A7
ATOM	2572		THR			-19.831	19.666	1.00	0.00	3A7
ATOM	2573	C	THR	363					0.00	3A7
MOTA	2574	0	THR	363	•	-19.042	18.805	1.00	0.00	3A7
ATOM	2575	N	LEU	364		-21.115	19.676	1.00		3A7
MOTA	2576	CA	LEU	364		-21.641	18.695	1.00	0.00	
ATOM	2577	СВ	LEU	364		-23.014	19.086	1.00	0.00	3A7
ATOM	2578	CG	LEU	364		-23.018	20.283	1.00	0.00	3A7
ATOM	2579		LEU	364		-24.462	20.696	1.00	0.00	3A7
ATOM	2580		LEU	364		-22.259	19.974	1.00	0.00	3A7
MOTA	2581	С	LEU	364		-21.746	17.338	1.00	0.00	3A7
MOTA	2582	0	LEU	364		-21.492	16.324	1.00	0.00	3A7
MOTA	2583	N	ARG	365		-22.094	17.264	1.00	0.00	3A7
MOTA	2584	CA	ARG	365	5.743	-22.109	16.003	1.00	0.00	. 3A7
MOTA	2585	СВ	ARG	365	4.300	-22.612	16.169	1.00	0.00	3A7
ATOM	2586	CG	ARG	365	3.614	-22.980	14.858	1.00	0.00	3A7
ATOM	2587	CD	ARG	365	2.117	-23.285	15.005	1.00	0.00	3A7
ATOM	2588	NE	ARG	365	1.371	-21.987	15.068	1.00	0.00	3A7
MOTA	2589	CZ	ARG	365		-21.942	15.201	1.00	0.00	3A7
ATOM	2590		ARG	365	-0.637	-20.742	15.124	1.00	0.00	3A7
ATOM	2591		ARG	365	-0.703	-23.084	15.418	1.00	0.00	3A7
ATOM	2592	С	ARG	365	5.648	-20.756	15.371	1.00	0.00	3A7
ATOM	2593	ō	λRG	365		-20.573	14.192	1.00	0.00	3A7 .
ATOM	2594	N	LEU	366		-19.760	16.176	1.00	0.00	3A7
ATOM	2595	CA	LEU	366		-18.410	15.729	1.00	0.00	3A7
ATOM	2596	CB	LEU	366		-17.608	16.752	1.00	0.00	3A7
ATOM	2597	CG	LEU	366		-16.833	16.122	1.00	0.00	3A7
ATOM	2598		LEU	366		-16.361	17.201	1.00	0.00	3A7
ATOM	2599	CD2		366		-15.648	15.240	1.00	0.00	3A7
ATOM	2600	C	LEU	366		-17.670	15.380	1.00	0.00	3A7
ATOM	2601	ŏ	LEU	366		-16.992	14.359	1.00	0.00	3A7
ATOM	2602	N	PHE	367		-17.798	16.193	1.00	0.00	3A7
						-17.136	15.897	1.00	0.00	3A7
ATOM	2603	CA	PHE	367					0.00	3A7
MOTA	2604	СВ	PHE	367		~16.072	16.907	1.00		3A7
MOTA	2605	CG	PHE	367		-15.081	17.042	1.00	0.00	
MOTA	2606		PHE	367		-15.250	18.035	1.00	0.00	3A7
MOTA	2607		PHE	367		-13.998	16.170	1.00	0.00	3A7
ATOM	2608		PHE	367		-14.365	18.137	1.00	0.00	3A7
ATOM	2609	CE2		367		-13.100	16.285	1.00	0.00	3A7
ATOM	2610	CZ	PHE	367		-13.284	17.269	1.00	0.00	3A7
MOTA	2611	С	PHE	367		-18.121	15.878	1.00	0.00	3A7
MOTA	2612	0	PHE	367		-18.207	16.823	1.00	0.00	3A7
ATOM	2613	N	PRO	368		-18.877	14.814	1.00	0.00	3A7
MOTA	2614	CA	PRO	368		-19.868	14.730	1.00	0.00	3A7
ATOM	2615	CD	PRO	368		-19.039	13.788	1.00	0.00	3A7
ATOM	2616	СВ	PRO	368	10.570	-20.710	13.544	1.00	0.00	3 <b>A</b> 7
ATOM	2617	CG	PRO	368	9.531	-19.942	12.757	1.00	0.00	3 <b>A</b> 7
ATOM	2618	С	PRO	368	12.257	-19.200	14.589	1.00	0.00	3 <b>A</b> 7
ATOM	2619	0	PRO	368	12.479	-18.434	13.657	1.00	0.00	3A7
ATOM	2620	N	VAL	369	13.143	-19.481	15.561	1.00	0.00	3 <b>A</b> 7

	ATOM	2621	CA	VAL	369	14.427	-18.858	15.709	1.00	0.00	3A7
	MOTA	2622	СВ	VAL	369		-19.329	16.991	1.00	0.00	3A7
	ATOM	2623 2624	CG1 CG2		369 369		-18.705 -18.876	17.115 18.133	1.00	0.00	3A7 3A7
	ATOM ATOM	2625	C	VAL	369		-19.141	14.529	1.00	0.00	3A7
	ATOM	2626	ō	VAL	369		-18.284	14.109	1.00	0.00	3A7
	ATOM	2627	N	ALA	370		-20.349	13.946	1.00	0.00	3A7
	ATOM	2628	CA	ALA	370		-20.686	12.775	1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2629 2630	CB C	ALA ALA	370 370		-22.035 -20.739	12.966 11.619	1.00	0.00	3A7
	ATOM	2631	ŏ	ALA	370		-21.792	11.309	1.00	0.00	3A7
	ATOM	2632	N	MET	371	14.813	-19.597	10.938	1.00	0.00	3A7
	MOTA	2633	CA	MET	371		-19.436	9.924	1.00	0.00	3A7 3A7
	ATOM	2634	CB	MET MET	371 371		-17.940 -17.053	9.616 9.800	1.00 1.00	0.00	3A7
	ATOM ATOM	2635 2636	CG SD	MET	371		-17.276	8.566	1.00	0.00	3A7
	ATOM	2637	CE	MET	371		-16.484	7.182	1.00	0.00	3A7
	ATOM	2638	С	MET	371		-20.142	8.625	1.00	0.00	3A7
	ATOM	2639	0	MET	371		-20.260	7.783	1.00	0.00	3A7 3A7
	ATOM	2640 2641	N CA	ARG ARG	372 372		-20.621 -21.368	8.432 7.254	1.00	0.00 0.00	3A7
	ATOM ATOM	2642	CB	ARG	372		-20.480	6.088	1.00	0.00	3A7
	ATOM	2643	CG	ARG	372		-19.769	5.248	1.00	0.00	3A7
	ATOM	2644	CD	ARG	372		-19.020	4.096	1.00	0.00	3A7
	ATOM	2645	NE	ARG	372		-18.673	2.996	1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2646 2647	CZ NH1	ARG	372 372		-19.599 -19.194	2.066 0.870	1.00	0.00	3A7
	ATOM	2648	NH2		372		-20.930	2.301	1.00	0.00	3A7
	ATOM	2649	C	ARG	372	16.832	-22.309	7.639	1.00	0.00	3A7
	MOTA	2650	0	ARG	372		-22.029	8.542	1.00	0.00	3A7
	ATOM	2651	N	LEU	373 373		-23.453 -24.462	6.907 7.034	1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2652 2653	CA CB	LEU	373		-25.879	7.360	1.00	0.00	3A7
	ATOM .	2654	CG	LEU	373		-26.016	8.700	1.00	0.00	3A7
	MOTA	2655	CD1	LEU	373		-25.305	9.860	1.00	0.00	3A7
	ATOM	2656	CD2		373		-25.605	8.611	1.00	0.00	3A7
	ATOM	2657 2658	С 0	LEU LEU	373 373		-24.532 -23.979	5.697 4.717	1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2659	N	GLU	374		-25.232	5.619	1.00	0.00	3A7
	ATOM	2660	CA	GLU	374		-25.477	4.356	1.00	0.00	3 <b>A</b> 7
	MOTA	2661	СВ	GLU	374		-24.637	4.153	1.00	0.00	3A7
	ATOM	2662	CG	GLU	374		-23.121	4.279	1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2663 2664	CD OE1	GLU	374 374		-22.422 -21.801	4.038 5.000	1.00	0.00	3A7
	ATOM	2665	OE2		374		-22.501	2.889	1.00	0.00	3A7
	ATOM	2666	С	GLU	374	20.862	-26.936	4.222	1.00	0.00	3A7
	MOTA	2667	0	GLU	374 .		-27.553	5.141	1.00	0.00	3A7
	ATOM	2668	N CA	ARG ARG	375 · 375		-27.510 -28.878	3.026 2.666	1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2669 2670	CB	ARG .	375		-29.770	2.636	1.00	0.00	3A7
	ATOM	2671	CG	ARG	375		-30.018	4.037	1.00	0.00	3A7
i	MOTA	2672	CD	ARG .	375		-30.919	4.035	1.00	0.00	3A7
	MOTA		NE	ARG	375		-31.381	5.436	1.00	0.00	3A7
	ATOM ATOM	2674 2675	CZ NH1	ARG	375 375		-30.590 -31.096	6.396 7.650	1.00	0.00 0.00	3A7 3A7
	ATOM	2676	NH2		375		-29.307	6.125	1.00	0.00	3A7
	MOTA	2677	С	ARG	375		-28.826	1.293	1.00	0.00	3A7
	MOTA	2678	0	ARG	375		-27.846	0.569	1.00	0.00	3A7
	ATOM	2679	N	VAL	376		-29.890	0.889 -0.420	1.00 1.00	0.00 0.00	3A7 3A7
	ATOM ATOM	2680 2681	CA CB	VAL VAL	376 376		-29.949 -29.725	-0.397	1.00	0.00	3A7
	MOTA	2682	CG1		376		-29.796	-1.822	1.00	0.00	3A7
i	ATOM	2683	CG2	VAL	376	24.638	-28.346	0.234	1.00	0.00	3A7
	MOŢA	2684	С	VAL	376		-31.316	-0.934	1.00	0.00	3A7
	ATOM ATOM	2685	O N	VAL CYS	376 377		-32.316 -31.397	-0.233 -2.212	1.00	0.00 0.00	3A7 3A7
	MOTA MOTA	2686 2687	CA	CYS	377		-32.642	-2.851	1.00	0.00	3A7
	ATOM	2688	СВ	CYS	377		-32.435	-4.083	1.00	0.00	3A7
į	MOTA	2689	SG	CYS	377		-31.876	-3.569	1.00	0.00	3A7
	ATOM	2690	C	CYS	377		-33.392	-3.254	1.00	0.00	3A7 3A7
	MOTA MOTA	2691 2692	И О	CYS LYS	377 378		-32.843 -34.705	-3.794 -2.955	1.00	0.00 0.00	3A7
- 4	W 1 O13	~ 0 7 4	44				3703	2.333	2.00		

MOTA	2693	CA	LYS	378	24.083	-35.594	-3.143	1.00	0.00	3A7
MOTA	2694	СВ	LYS	378		-36.718	-2.075	1.00	0.00	3A7
MOTA	2695	CG	LYS	378		-36.428	-0.894	1.00	0.00	3A7 3A7
MOTA MOTA	2696 2697	CD CE	LYS LYS	378 378		-37.592 -37.375	0.101 1.174	1.00	0.00	3A7
ATOM	2698	NZ	LYS	378		-36.159	1.974	1.00	0.00	3A7
ATOM	2699	c	LYS	378		-36.202	-4.524	1.00	0.00	3A7
MOTA	2700	0	LYS	378		-36.609	-5.075	1.00	0.00	3A7
ATOM	2701	N	LYS	379		-36.285	-5.081	1.00	0.00	3A7
ATOM	2702	CA	LYS	379		-36.939	-6.329	1.00	0.00	3A7
ATOM ATOM	2703 2704	CB CG	LYS LYS	379 379		-38.417 -38.609	-6.127 -5.161	1.00	0.00 0.00	3A7 3A7
ATOM	2704	CD	LYS	379		-40.083	-4.899	1.00	0.00	3A7
ATOM	2706	CE	LYS	379		-40.842	-4.120	1.00	0.00	3A7
MOTA	2707	NZ	LYS	379	21.236	-42.233	-3.850	1.00	0.00	3A7
ATOM	2708	C	LYS	379		-36.155	-6.981	1.00	0.00	3A7
ATOM	2709	0	LYS	379		-35.119 -36.650	-6.483 -8.134	1.00	0.00	3A7 3A7
ATOM ATOM	2710 2711	N CA	ASP ASP	380 380		-36.071	-8.818	1.00	0.00	3A7
ATOM	2712	СВ	ASP	380		-36.404		1.00	0.00	3A7
ATOM	2713	CG	ASP	380		-35.921		1.00	0.00	3A7
MOTA	2714		ASP	380		-34.689		1.00	0.00	3A7
ATOM	2715		ASP	380		-36.782		1.00	0.00	3A7 3A7
ATOM ATOM	2716 2717	C O	ASP ASP	380 380		-36.616 -37.798	-8.182 -7.848	1.00	0.00	3A7
ATOM	2718	N	VAL	381		-35.744	-7.966	1.00	0.00	3A7
ATOM	2719	CA	VAL	381		-36.118	-7.224	1.00	0.00	3A7
ATOM	2720	СВ	VAL	381		-35.910	-5.720	1.00	0.00	3A7
ATOM	2721		VAL	381		-34.439	-5.360	1.00	0.00	3A7
ATOM	2722	CG2 C	VAL	381		-36.489 -35.308	-4.947 -7.781	1.00	0.00	3A7 3A7
ATOM ATOM	2723 2724	ò	VAL	381 381		-34.151	-8.142	1.00	0.00	3A7
ATOM	2725	N	GLU	382		-35.908	-7.874	1.00	0.00	3A7
ATOM	2726	ÇA	GLU	382	12.888	-35.247	-8.420	1.00	0.00	3A7
ATOM	2727	СВ	GLU	382		-36.100	-9.485	1.00	0.00	3A7
ATOM	2728	CG	GLU	382		-36.325		1.00	0.00	3A7 3A7
ATOM ATOM	2729 2730	CD OE1	GLU GLU	382 382		-37.311 -38 470	-10.571	1.00	0.00	3A7
ATOM	2731		GLU	382			-10.822	1.00	0.00	3A7
ATOM	2732	С	GLU	382		-34.980	-7.271	1.00	0.00	3A7
ATOM	2733	0	GLU	382		-35.909	-6.587	1.00	0.00	3A7
ATOM	2734 2735	N	ILE	383 383		-33.690 -33.270	-7.028 -5.937	1.00	0.00	3A7 3A7
ATOM ATOM	2736	CA CB	ILE	383		-32.299	-4.973	1.00	0.00	3A7
ATOM	2737		ILE	383		-32.043	-3.747	1.00	0.00	3A7
ATOM	2738	CG1	ILE	383	12.865	-32.774	-4.555	1.00	0.00	3A7
ATOM	2739	CD	ILE	383		-34.026	-3.677	1.00	0.00	3A7
ATOM	2740 2741	C	ILE	383 383		-32.594 -31.493	-6.567 -7.103	1.00	0.00	3A7 . 3A7
ATOM ATOM	2742	O. N	ILE ASN	384		-33.254	-6.521	1.00	0.00	3A7
ATOM	2743	CA	ASN	384		-32.719	-6.976	1.00	0.00	. 3A7
ATOM	2744	CB	ASN	384	6.732	-31.411	-6.222	1.00	0.00	3A7
ATOM	2745	CG	ASN	384		-31.147	-6.283	1.00	0.00	3A7
ATOM	2746		ASN	384			-7.000	1.00	0.00	3A7 3A7
ATOM ATOM	2747 2748	C	ASN ASN	384 384		-31.956 -32.504	-5.498 -8.480	1.00	0.00	3A7
ATOM	2749	ŏ	ASN	384		-31.623	-8.988	1.00	0.00	3A7
ATOM	2750	N	GLY	385		-33.322	-9.231	1.00	0.00	3A7
ATOM	2751	CA	GLY	385			-10.666	1.00	0.00	3A7
ATOM ATOM	2752	C	GLY	385			-11.156	1.00	0.00	3A7 3A7
ATOM	2753 2754	O N	GLY MET	385 386			-12.366 -10.264	1.00	0.00	3A7
ATOM	2755	CA	MET	386			-10.695	1.00	0.00	3A7
ATOM	2756	СВ	MET	386			-10.426	1.00	0.00	3A7
MOTA	2757	CG	MET	386		-28.845	-8.990	1.00	0.00	3A7
ATOM	2758	SD	MET	386		-27.091	-8.895	1.00	0.00	3A7
ATOM ATOM	2759 2760	CE C	MET MET	386 386		-26.373 -31 305	-9.388 -10.187	1.00	0.00	3A7 3A7
ATOM	2761	0	MET	386		-31.654	-9.025	1.00	0.00	3A7
ATOM	2762	N	PHE	387			-11.125	1.00	0.00	3A7
ATOM	2763	CA	PHE	387			-10.982	1.00	0.00	3A7
MOTA	2764	СВ	PHE	387	14.935	-32.474	-12.378	1.00	0.00	3A7

ATOM	2765	CG	PHE	387	14.10	2 -33.505	-13.091	1.00	0.00	3A7
ATOM	2766		PHE	387	14.64	-34.767	-13.344	1.00	0.00	3A7
ATOM	2767		PHE	387	12.82	7 -33.213	-13.585	1.00	0.00	3A7
ATOM	2768		PHE	387		-35.727		1.00	0.00	3A7
ATOM	2769		PHE	387		7 -34.173	_	1.00	0.00	3A7
ATOM	2770	CZ	PHE	387		2 -35.433		1.00	0.00	3A7
ATOM	2771	c	PHE	387		5 -31.180		1.00	0.00	3A7
ATOM	2772	ō	PHE	387		L -30.043		1.00	0.00	3A7
	2773	N	ILE	388		6 -31.706	-9.251	1.00	0.00	3A7
ATOM			ILE	388		5 -31.049	-8.544	1.00	0.00	3A7
ATOM	2774	CA				4 -31.071	-7.032	1.00	0.00	3A7
MOTA	2775	CB	ILE	388		4 -30.276	-6.387	1.00	0.00	3A7
ATOM	2776		ILE	388				1.00	0.00	3A7
ATOM	2777		ILE	388		1 -30.487	-6.591	1.00	0.00	3A7
ATOM	2778	CD	ILE	388		4 -29.010	-6.913			
ATOM	2779	C	ILE	388		8 -31.746		1.00	0.00	3A7 3A7
ATOM	2780	0	ILE	388		6 -32.952	-8.728	1.00	0.00	
ATOM	2781	N	PRO	389		5 -31.021	-9.496	1.00	0.00	3A7
MOTA	2782	ÇA	PRO	389		8 -31.581	-9.867	1.00	0.00	3A7
MOTA	2783	CD	PRO	389		3 -29.901		1.00	0.00	3A7
MOTA	2784	СВ	PRO	389		0 -30.549		1.00	0.00	3A7
ATOM	2785	CG	PRO	389		1 -29.931		1.00	0.00	3A7
ATOM	2786	С	PRO ·	389		4 -31.785	-8.684	1.00	0.00	3A7
ATOM	2787	0	PRO	389	21.47	4 -31.121	-7.659	1.00	0.00	3A7
ATOM	2788	N	LYS	390	22.62	7 -32.663	-8.836	1.00	0.00	3A7
ATOM	2789	CA	LYS	390	23.65	4 -32.884	-7.847	1.00	0.00	3A7
ATOM	2790	ÇВ	LYS	390	24.73	3 -33.851	-8.363	1.00	0.00	3A7
ATOM	2791	CG	LYS	390	24.23	4 -35.053	-9.176	1.00	0.00	3A7
ATOM	2792	CD	LYS	390	25.37	2 -36.029	-9.517	1.00	0.00	3A7
ATOM	2793	CE	LYS	390	24.92	1 -37.258	-10.316	1.00	0.00	3A7
ATOM	2794	NZ	LYS	390	23.95	9 -38.073	-9.538	1.00	0.00	3A7
ATOM	2795	С	LYS	390	24.34	6 -31.584	-7.486	1.00	0.00	3A7
ATOM	2796	Ô	LYS	390	24.63	1 -30.776	-8.366	1.00	0.00	3A7
ATOM	2797	N	GLY	391	24.55	8 -31.329	-6.177	1.00	0.00	3A7
ATOM	2798	CA	GLY	391		0 -30.153	-5.707	1.00	0.00	3A7
ATOM	2799	C	GLY	391		7 -28.926	-5.567	1.00	0.00	3A7
ATOM	2800	ŏ	GLY	391		4 -27.848		1.00	0.00	3A7
ATOM	2801	N	VAL	392		2 -29.029		1.00	0.00	3A7
ATOM	2802	CA	VAL	392		9 -27.896		1.00	0.00	3A7
ATOM	2803	СВ	VAL	392		9 -28.126		1.00	0.00	3A7
ATOM	2804		VAL	392		5 -27.062	-5.883	1.00	0.00	3A7
ATOM	2805		VAL	392		4 -28.134	-7.744	1.00	0.00	3A7
ATOM	2806	C	VAL	392		2 -27.684	-4.050	1.00	0.00	3A7
ATOM	2807	ō	VAL	392		9 -28.644	-3.290	1.00	0.00	3A7
	2808	N	VAL	393		7 -26.403		1.00	0.00	3A7
ATOM	2809	CA	VAL	393		1 -26.024	-2.268	1.00	0.00	3A7
MOTA			VAL	393		B -24.695	-1.900	1.00	0.00	3A7
ATOM	2810	CB CG1	VAL	393		B -24.336		1.00	0.00	3A7
ATOM ATOM	2811		VAL	393		6 -24.785		1.00	0.00	3A7
	2812			393		2 -25.964	-2.130	1.00	0.00	3A7
ATOM	2813	C	VAL		•	8 -25.288		1.00	0.00	3A7
ATOM	2814	0	VAL	393		7 <b>-</b> 26.712		1.00	0.00	3A7
ATOM	2815	N	VAL	394				1.00	0.00	3A7
ATOM	2816	CA	VAL	394		9 -26.825			0.00	3A7
ATOM	2817	CB	VAL	394		9 -28.282		1.00	0.00	3A7
ATOM	2818		VAL	394		4 -28.411		1.00	0.00	3A7
ATOM	2819		VAL	394		8 -28.936				3A7
ATOM	2820	C	VAL	394		0 -26.177		1.00	0.00	3A7
ATOM	2821	0	VAL	394		1 -26.423		1.00	0.00	
ATOM	2822	N	MET	395		0 -25.325		1.00	0.00	3A7
MOTA	2823	CA	MET	395		9 -24.656		1.00	0.00	3A7
ATOM	2824	СВ	MET	395		8 -23.145		1.00	0.00	3A7
ATOM	2825	CG	MET	395		4 -22.812		1.00	0.00	3A7
ATOM	2826	SD	MET	395		7 -21.101		1.00	0.00	3A7
ATOM	2827	CE	MET	395	-	0 -20.277		1.00	0.00	3A7
ATOM	2828	С	MET	395		3 -24.885		1.00	0.00	3A7
ATOM	2829	0	MET	395		5 -24.925		1.00	0.00	3A7
ATOM	2830	N	ILE	396		2 -25.076		1.00	0.00	3A7
ATOM	2831	CA	ILE	396		6 -25.356		1.00	0.00	3A7
MOTA	2832	CB	ILE	396		9 -26.610		1.00	0.00	3A7
MOTA	2833	CG2	ILE	396		0 -26.667		1.00	0.00	3A7
ATOM	2834	CG1	ILE	396		9 -27.897		1.00	0.00	3A7
ATOM	2835	CD	ILE	396	15.08	7 -28.104		1.00	0.00	3A7
ATOM	2836	С	ILE	396	13.18	8 -24.182	4.902	1.00	0.00	3A7
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ATOM	2837	0	ILE	396	13.874	-23.964	5.894	1.00	0.00	3A7
ATOM	2838	N	PRO	397		-23.398	4.590	1.00	0.00	3A7
ATOM	2839	CA	PRO	397		-22.297	5.462	1.00	0.00	3A7
MOTA	2840	CD CB	PRO PRO	397 397		-23.022 -21.252	3.209 4.533	1.00	0.00	3A7 3A7
MOTA MOTA	2841 2842	CG	PRO	397		-22.043	3.293	1.00	0.00	3A7
ATOM	2843	ç	PRO	397		-22.717	6.544	1.00	0.00	3A7
ATOM	2844	0	PRO	397	9.629	-22.732	6.310	1.00	0.00	3A7
ATOM	2845	N	SER	398		-22.981	7.767	1.00	0.00	3A7
ATOM	2846	CA	SER	398		-23.392	8.914	1.00	0.00	3A7 3A7
ATOM ATOM	2847 2848	CB OG	SER	398 398		-23.676 -22.517	10.138 10.613	1.00	0.00	3A7
ATOM	2849	c	SER	398		-22.379	9.316	1.00	0.00	3A7
ATOM	2850	ō	SER	398		-22.745	9.668	1.00	0.00	3A7
ATOM	2851	N	TYR	399		-21.053	9.231	1.00	0.00	3A7
ATOM	2852	CA	TYR	399		-19.958	9.507	1.00	0.00	3A7
ATOM	2853	CB CG	TYR TYR	399 399		-18.562 -17.492	9.264 10.212	1.00 1.00	0.00	3A7 3A7
ATOM ATOM	2854 2855		TYR	399		-16.936	11.172	1.00	0.00	3A7
ATOM	2856		TYR	399		-17.008	10.123	1.00	0.00	3A7
ATOM	2857	CE1	TYR	399		-15.959	12.051	1.00	0.00	3A7
ATOM	2858		TYR	399		-16.041	11.007	1.00	0.00	3A7
ATOM	2859	CZ	TYR	399		-15.520 -14.553	11.975 12.880	1.00	0.00	3A7 3A7
ATOM ATOM	2860 2861	OH C	TYR TYR	399 399		-20.038	8.647	1.00	0.00	3A7
ATOM	2862	ō	TYR	399		-19.765	9.067	1.00	0.00	3A7
MOTA	2863	N	VAL	400		-20.472	7.398	1.00	0.00	3A7
MOTA	2864	CA	VAL	400		-20.616	6.436	1.00	0.00	3A7
ATOM	2865	CB	VAL	400		-20.658	5.045	1.00	0.00	. 3A7 3A7
ATOM ATOM	2866 2867	CG1		400 400		-20.758 -19.308	4.020 4.899	1.00	0.00	3A7
ATOM	2868	C	VAL	400		-21.827	6.653	1.00	0.00	3A7
ATOM	2869	0	VAL	400	4.781	-21.734	6.547	1.00	0.00	3A7
ATOM	2870	N	LEU	401		-22.992	6.970	1.00	0.00	3A7
ATOM	2871	CA	LEU	401		-24.224	7.175	1.00	0.00	3A7
ATOM ATOM	2872 2873	CB CG	LEU	401 401		-25.449 -25.453	7.318 6.535	1.00	0.00	3A7 3A7
ATOM	2874	CD1		401		-26.722	6.915	1.00	0.00	3A7
ATOM	2875	CD2		401		-25.294	5.023	1.00	0.00	3A7
MOTA	2876	С	LEU	401		-24.186	8.449	1.00	0.00	3A7
ATOM	2877	0	LEU	401		-24.705	8.504	1.00	0.00	3A7
ATOM .	2878 2879	N CA	HIS HIS	402 402		-23.512 -23.303	9.509 10.782	1.00	0.00	3A7 3A7
ATOM .	2880	ND1		402		-24.809	12.042	1.00	0.00	3A7
ATOM	2881	CG	HIS	402		-23.553	12.480	1.00	0.00	3A7
ATOM	2882	СВ	HIS	402		-22.628	11.778	1.00	0.00	3A7
ATOM	2883	NE2		402		-24.122	13.375	1.00	0.00	3A7
MOTA	2884 2885	CD2		402 402		-23.155 -25.085	13.305 12.595	1.00	0.00	3A7 3A7
ATOM	2886	CEI	HIS	402		-22.420	10.674	1.00	0.00	3A7
ATOM	2887	ō.	HIS	402		-22.343	11.602	1.00	0.00	3A7
MOTA	2888	N	HIS	403		-21.730	9.522	1.00	0.00	3A7
ATOM	2889	CA	HIS	403		-20.839	9.280	1.00	0.00	3A7
MOTA MOTA	2890 2891	ND1 CG	HIS	403 403		-19.115 -18.746	10.966 10.299	1.00	0.00	3A7 3A7
ATOM	2892	CB	HIS	403		-19.394	9.048	1.00	0.00	3A7
ATOM	2893	NE2		403		-17.451	12.131	1.00	0.00	3A7
ATOM	2894	CD2		403		-17.730	11.028	1.00	0.00	3A7
ATOM	2895	CEI		403		-18.308	12.051	1.00	0.00	3A7
ATOM ATOM	2896 2897	С 0	HIS HIS	403 403		-21.280 -20.492	8.096 7.500	1.00	0.00	3A7 3A7
ATOM	2897	N	ASP	403		-22.588	7.740	1.00	0.00	3A7
ATOM	2899	CA	ASP	404		-23.143	6.662	1.00	0.00	3A7
ATOM	2900	СВ	ASP	404		-24.585	6.322	1.00	0.00	3A7
ATOM	2901	CG	ASP	404		-25.218	5.103	1.00	0.00	3A7
ATOM	2902		ASP	404		-24.540 -26.417	4.402 4.850	1.00	0.00	3A7 3A7
MOTA MOTA	2903 2904	C C	ASP ASP	404 404		-26.417	7.105	1.00	0.00	3A7
ATOM	2905	ŏ	ASP	404		-23.809	8.108	1.00	0.00	3A7
MOTA	2906	N	PRO	405		-22.474	6.421	1.00	0.00	3A7
MOTA	2907	CA	PRO	405		-22.344	6.827	1.00	0.00	3A7
ATOM	2908	CD	PRO	405	-1.277	-21.674	5.237	1.00	0.00	3A7

ATOM	2909	СВ	PRO	405	-3 543	-21.309	5.854	1.00	0.00	3A7
MOTA	2910	CG	PRO	405	-2.641	-21.373	4.621	1.00	0.00	3A7
ATOM	2911	С	PRO	405	-3.739	-23.646	6.756	1.00	0.00	3A7
ATOM	2912	0	PRO	405	-4 766	-23.734	7.420	1.00	0.00	3A7
ATOM	2913	N	LYS	406	-3.297	-24.674	5.989	1.00	0.00	3A7
MOTA	2914	CA	LYS	406	-3.983	-25.942	5.892	1.00	0.00	. 3A7
MOTA	2915	СВ	LYS	406		-26.748	4.646	1.00	0.00	3A7
ATOM	2916	CG	LYS	406	-3.805	-26.004	3.326	1.00	0.00	3A7
ATOM	2917	CD	LYS	406	-3.234	-26.692	2.072	1.00	0.00	3a7
ATOM	2918	CE	LYS	406		-27.993	1.650	1.00	0.00	3A7
ATOM	2919	NZ	LYS	406	-3.601	-29.127	2.541	1.00	0.00	3A7
ATOM	2920	С	LYS	406	-3.730	-26.791	7.115	1.00	0.00	3A7
ATOM	2921	0	LYS	406	-4 554	-27.622	7.479	1.00	0.00	3A7
ATOM	2922	N	TYR	407	-2.5/2	-26.584	7.783	1.00	0.00	3A7
ATOM	2923	CA	TYR	407	-2.174	-27.340	8.948	1.00	0.00	3A7
ATOM	2924	СВ	TYR	407	-0.677	-27.703	8.898	1.00	0.00	3A7
						-28.906			0.00	3A7
MOTA	2925	CG	TYR	407			8.000	1.00		
ATOM	2926	CD1	TYR	407	-0.674	-28.783	6.613	1.00	0.00	3A7
ATOM	2927	CD2	TYR	407	-0.492	-30.184	8.557	1.00	0.00	3A7
						-29.912	5.799	1.00	0.00	3A7
ATOM	2928		TYR	407						
ATOM	2929	CE2	TYR	407	-0.483	-31.314	7.746	1.00	0.00	3A7
ATOM	2930	CZ	TYR	407	-0.585	-31.179	6.365	1.00	0.00	3A7
	2931	ОН	TYR	407		-32.324	5.538	1.00	0.00	3A7
ATOM										
ATOM	2932	С	TYR	407	-2.474	-26.584	10.218	1.00	0.00	3A7
ATOM	2933	0	TYR	407	-2.827	-27.189	11.229	1.00	0.00	3A7
	2934					-25.240	10.202	1.00	0.00	3A7
ATOM		N	TRP	408						
MOTA	2935	CA	TRP	408	-2.553	-24.414	11.368	1.00	0.00	3A7
ATOM	2936	CB	TRP	408	-1.243	-23.786	11.891	1.00	0.00	3A7
ATOM	2937	CG	TRP	408		-24.837	12.291	1.00	0.00	3A7
ATOM	2938	CD2	TRP	408	-0.524	-25.818	13.304	1.00	0.00	3A7
ATOM	2939	CD1	TRP	408	1.005	-25.107	11.823	1.00	0.00	3A7
ATOM	2940	NE1	TRP	408	1.515	-26.195	12.482	1.00	0.00	3A7
ATOM	2941		TRP	408		-26.677	13.353	1.00	0.00	3A7
ATOM	2942	CE3	TRP	408	-1.619	-26.011	14.121	1.00	0.00	3A7
ATOM	2943	CZ2	TRP	408	0.578	-27.783	14.170	1.00	0.00	3A7
							14.983	1.00	0.00	3A7
ATOM.	2944		TRP	408		-27.102				
ATOM	2945	CH2	TRP	408	-0.524	-27.989	14.995	1.00	0.00	3A7
ATOM	2946	С	TRP	408 -	-3.541	-23.347	10.974	1.00	0.00	3A7
ATOM	2947	0	TRP	408		-22.324	10.383	1.00	0.00	3A7
MOTA	2948	N	THR	409		-23.556	11.320	1.00	0.00	3A7
ATOM	2949	CA	THR	409	-5.897	-22.587	11.078	1.00	0.00	3A7
ATOM	2950	СВ	THR	409		-23.197	11.275	1.00	0:00	3A7
										3A7
MOTA	2951		THR	409		-22.316	10.873	1.00	0.00	
ATOM	2952	CG2	THR	409	-7.503	-23.671	12.727	1.00	0.00	3A7
ATOM	2953	Ċ	THR	409	-5.686	-21.354	11.951	1.00	0.00	3A7
ATOM	2954	ō		409		-21.439	13.116	1.00	0.00	3A7
			THR							
MOTA	2955	N	GLU	410	-5.888	-20.153	11.363	1.00	0.00	3A7
ATOM	2956	CA	GLU	410	-5.519	-18.880	11.957	1.00	0.00	3A7
ATOM	2957	СВ	GLU	410		-18.485	13.138	1.00	0.00	3A7
				-						
ATOM	2958	CG	GLU	410		-18.447	12.751	1.00	0.00	3A7
ATOM	2959	CD	GLU	410	-8.744	-18.043	13.970	1.00	0.00	3A7
ATOM	2960	OE1	GLU	410	-8.705	-18.790	14.985	1.00	0.00	3A7
ATOM	2961		GLU	410		-16.984	13.903	1.00	0.00	3A7
ATOM	2962	С	GLU	410	-4.059	-18.872	12.399	1.00	0.00	3A7
ATOM	2963	0	GLU	410	-3.756	-18.654	13.572	1.00	0.00	3A7
ATOM	2964	N	PRO	411		-19.188	11.476	1.00	0.00	3A7
						-19.438	11.747		0.00	3A7
ATOM	2965	CA	PRO	411				1.00		
ATOM	2966	CD	PRO	411	-3.394	-19.045	10.041	1.00	0.00	3A7
ATOM	2967	СВ	PRO	411	-1.144	-19.794	10.370	1.00	0.00	3A7
ATOM	2968	CG	PRO	411		-19.039	9.368	1.00	0.00	3A7
ATOM	2969	С	PRO	411		-18.216	12.290	1.00	0.00	3A7
MOTA	2970	0	PRO	411	0.020	-18.335	12.931	1.00	0.00	3A7
ATOM	2971	N	GLU	412	-1.592	-17.019	12.058	1.00	0.00	3A7
									0.00	3A7
ATOM	2972	CA	GLU	412		-15.791	12.493	1.00		
ATOM	2973	CB	GLU	412	-1.368	-14.650	11.516	1.00	0.00	3A7
MOTA	2974	CG	GLU	412	-0.914	-14.895	10.063	1.00	0.00	3A7
ATOM	2975	CD	GLU	412		-14.849	9.920	1.00	0.00	3A7
ATOM	2976	OE1		412		-15.190	8.807	1.00	0.00	3A7
MOTA	2977	OE2	GLU	412	1.306	-14.468	10.897	1.00	0.00	3A7
ATOM	2978	С	GLU	412		-15.419	13.903	1.00	0.00	3A7
										3A7
ATOM	2979	0	GLU	412		-14.360	14.405	1.00	0.00	
ATOM	2980	N	LYS	413	-2.226	-16.290	14.589	1.00	0.00	3A7

ATOM	2981	CA	LYS	413	-2.691	-16.035	15.932	1.00	0.00	3A7
ATOM	2982	СВ	LYS	413		-16.281	16.093	1.00	0.00	3A7
ATOM	2983	CG	LYS	413		-15.300	15.276	1.00	0.00	3A <b>7</b>
ATOM	2984	CD	LYS	413		-15.457	15.519	1.00	0.00	3A7
ATOM	2985	CE	LYS	413		-15.075	16.938	1.00	0.00	3A7
ATOM	2986	NZ	LYS	413		-15.230	17.084	1.00	0.00	3A7
ATOM	2987	С	LYS	413		-16.896	16.917	1.00	0.00	3A7
ATOM	2988	o	LYS	413		-18.089	16.718	1.00	0.00	3A7
ATOM	2989	N	PHE	414		-16.288	18.059	1.00	0.00	3A7
ATOM	2990	CA	PHE	414		-16.968	19.200	1.00	0.00	3A7
ATOM	2991	СВ	PHE	414		-15.950	20.125	1.00	0.00	3A7
ATOM	2992	CG	PHE	414		-16.580	21.179	1.00	0.00	3A7
ATOM	2993		PHE	414		-17.214	20.878	1.00	0.00	3A7
ATOM	2994		PHE	414	0.126	-16.541	22.505	1.00	0.00	3A7
ATOM	2995		PHE	414	2.507	-17.815	21.887	1.00	0.00	3A7
ATOM	2996	CE2	PHE	414	0.864	-17.148	23.513	1.00	0.00	3A <b>7</b>
ATOM	2997	CZ	PHE	414	2.048	-17.802	23.199	1.00	0.00	3A7
ATOM	2998	С	PHE	414	-2.045	-17.668	19.981	1.00	0.00	3A7
ATOM	2999	0	PHE	414	-2.819	-17.039	20.697	1.00	0.00	3A7
ATOM	3000	N	LEU	415	-2.093	-19.006	19.847	1.00	0.00	3A7
ATOM	3001	CA	LEU	415	-3.087	-19.816	20.488	1.00	0.00	3A7
ATOM	3002	СВ	LEU	415	-4.201	-20.254	19.504	1.00	0.00	3A7
ATOM	3003	CG	LEU	415	-5.081	-19.105	18.954	1.00	0.00	3A7
ATOM	3004	CD1	LEU	415	-5.988	-19.603	17.812	1.00	0.00	3 <b>a7</b>
ATOM	3005	CD2	LEU	415	-5.911	-18.424	20.058	1.00	0.00	3A7
ATOM	3006	С	LEU	415	-2.421	-21.064	20.998	1.00	0.00	3A7
ATOM	3007	0	LEU	415	-2.308	-22.038	20.252	1.00	0.00	3A7
ATOM	3008	N	PRO	416	-2.010	-21.141	22.271	1.00	0.00	3A7
ATOM	3009	CA	PRO	416	-1.339	-22.301	22.847	1.00	0.00	3A7
ATOM	3010	CD	PRO	416	-1.874	-19.967	23.122	1.00	0.00	3A7
ATOM	3011	СВ	PRO	416	-1.071	-21.888	24.299	1.00	0.00	3A7
ATOM	3012	CG	PRO	416		-20.375	24.207	1.00	0.00	3A7
MOTA	3013	С	PRO	416		-23.547	22.780	1.00	0.00	3A7
MOTA	3014	0	PRO	416		-24.651	22.766	1.00	0.00	3A7
ATOM	3015	N	GLU	417		-23.381	22.682	1.00	0.00	3A7
ATOM	3016	CA	GLU	417		-24.458	22.678	1.00	0.00	3A7
ATOM	3017	CB	GLU	417		-23.933	22.878	1.00	0.00	3A7
ATOM	3018	CG	GLU	417		-23.126	24.179	1.00	0.00	3A7
MOTA	3019	CĐ	GLU	417		-22.672	24.323	1.00	0.00	3A7
MOTA	3020		GLU	417		-23.077	25.322	1.00	0.00	3A7
ATOM	3021		GLU	417		-21.911		1.00	0.00	3A7
MOTA	3022	С	GLU	417		-25.295	21.427	1.00	0.00	3A7
ATOM	3023	.0	GLU	417			21.478	1.00	0.00	3A7
ATOM	3024	N	ARG	418		-24.733	20.282	1.00	0.00	3A7
ATOM	3025	CA	ARG	418		-25.279	18.944	1.00	0.00	3A7
ATOM	3026	CB	ARG	418		-24.206	17.890	1.00	0.00	3A7 3A7
ATOM	3027	CG	ARG	418		-24.508	16.422	1.00	0.00	3A7
ATOM	3028	CD	ARG	418		-24.343	16.069	1.00	0.00	3A7
ATOM	3029	NE	ARG	418		-25.466	16.668	1.00	0.00	3A7
ATOM	3030 3031	CZ	ARG	418		-25.471 -26.503	16.670 17.264	1.00	0.00	3A7
ATOM	3031		ARG ARG	418 418		-24.456	16.087	1.00	0.00	3A7
ATOM	3032	C	ARG	418		-26.538	18.706	1.00	0.00	3A7
ATOM	3033	Ö	ARG	418		-26.489	18.187	1.00	0.00	3A7
ATOM ATOM	3035	N	PHE	419		-27.699	19.103	1.00	0.00	3A7
ATOM	3036	CA	PHE	419		-29.076	18.984	1.00	0.00	3A7
ATOM	3037	СВ	PHE	419		-29.565	17.516	1.00	0.00	3A7
ATOM	3038	CG	PHE	419		-29.517	16.915	1.00	0.00	3A7
ATOM	3039		PHE	419		-28.723	15.799	1.00	0.00	3A7
ATOM	3040		PHE	419		-30.278	17.466	1.00	0.00	3A7
ATOM	3041		PHE	419		-28.691	15.246	1.00	0.00	3A7
ATOM	3042		PHE	419		-30.245	16.919	1.00	0.00	3A7
ATOM	3043	cz	PHE	419		-29.452	15.806	1.00	0.00	3A7
ATOM	3044	c	PHE	419		-29.334	19.681	1.00	0.00	3A7
ATOM	3045	ŏ	PHE	419		-28.961	19.199	1.00	0.00	3A7
ATOM	3046	N	SER	420		-30.000	20.861	1.00	0.00	3A7
ATOM	3047	CA	SER	420		-30.259	21.764	1.00	0.00	3A7
ATOM	3048	СВ	SER	420		-30.137	23.241	1.00	0.00	3A7
ATOM	3049	ŌĞ	SER	420		-30.208	24.172	1.00	0.00	3A7
ATOM	3050	c	SER	420		-31.644	21.508	1.00	0.00	3A7
ATOM	3051	0	SER	420		-32.527	21.013	1.00	0.00	3A7
MOTA	3052	N	LYS	421		-31.842	21.877	1.00	0.00	3A7

ATOM	3053	CA	LYS	421	1.404	-33.112	21.813	1.00	0.00	3A7
ATOM	3054	СВ	LYS	421		-33.196	20.717	1.00	0.00	3A7
ATOM	3055	CG	LYS	421	3.804	-32.380	20.921	1.00	0.00	3A7
MOTA	3056	CD	LYS	421		-30.845	20.996	1.00	0.00	3A7
MOTA	3057	CE	LYS	421		-30.147	19.673	1.00	0.00	3A7
MOTA	3058	NZ	LYS	421		-30.385	19.273	1.00	0.00	3A7
ATOM	3059	С	LYS	421		-33.350	23.167	1.00	0.00	3A7 3A7
ATOM	3060	0	LYS	421		-32.424	23.962	1.00	0.00 0.00	3A7
ATOM	3061	N	LYS	422		-34.620 -34.986	23.448 24.675	1.00	0.00	3A7
ATOM	3062 3063	CA CB	LYS LYS	422 422		-35.203	25.856	1.00	0.00	3A7
MOTA MOTA	3064	CG	LYS	422		-35.433	27.225	1.00	0.00	3A7
ATOM	3065	CD	LYS	422		-34.222	27.727	1.00	0.00	3A7
ATOM	3066	CE	LYS	422		-34.436	29.109	1.00	0.00	3A7
ATOM	3067	NZ	LYS	422		-35.537	29.071	1.00	0.00	3A7
ATOM	3068	C	LYS	422		-36.262	24.379	1.00	0.00	3A7
ATOM	3069	0	LYS	422	4.874	-36.483	24.867	1.00	0.00	3A7
ATOM	3070	N	ASN	423	3.138	-37.137	23.555	1.00	0.00	3A7
ATOM	3071	CA	ASN	423	3.658	-38.427	23.165	1.00	0.00	3A7
ATOM	3072	CB	ASN	423		-39.581	23.442	1.00	0.00	3A7
ATOM	3073	CG	ASN	423		-39.329	22.812	1.00	0.00	3A7
MOTA	3074		ASN	423		-38.476	23.277	1.00	0.00	3A7
ATOM	3075		ASN	423		-40.110	21.734	1.00	0.00	3A7 3A7
ATOM	3076	C	ASN	423		-38.367	21.703	1.00	0.00	3A7 3A7
ATOM	3077	0	ASN	423		-37.323 -39.522	21.061 21.148	1.00	0.00	. 3A7
ATOM	3078	N	LYS	424 424		-39.522	19.760	1.00	0.00	3A7
ATOM ATOM	3079 3080	CA CB	LYS LYS	424		-40.724	19.591	1.00	0.00	3A7
ATOM	3081	CG	LYS	424		-40.859	18.153	1.00	0.00	3A7
ATOM	3082	CD	LYS	424		-41.874	18.013	1.00	0.00	3A7
ATOM	3083	CE	LYS	424		-41.460	18.744	1.00	0.00	3A7
ATOM	3084	NZ	LYS	424	10.027	-42.465	18.534	1.00	0.00	3A7
ATOM	3085	C	LYS	424		-40.125	18.981	1.00	0.00	3A7
MOTA	3086	0	LYS	424		-41.116	19.335	1.00	0.00	3A7
MOTA	3087	N	ASP	425		-39.353	17.910	1.00	0.00	3A7
ATOM	3088	CA	ASP	425		-39.492	17.032	1,00	0.00	3A7
ATOM	3089	CB	ASP	425		-40.959	16.658	1.00	0.00	3A7 3A7
ATOM	3090	CG	ASP	425		-41.005	15.496	1.00	0.00	3A7 3A7
ATOM	3091		ASP ASP	425		-41.550 -40.497	15.698 14.397	1.00	0.00	3A7
ATOM ATOM	3092 3093	C	ASP	425 425		-38.771	17.679	1.00	0.00	3A7
ATOM	3094	o	ASP	425		-39.355	18.444	1.00	0.00	3A7
ATOM	3095	N	ASN	426		-37.457	17.372	1.00	0.00	3A7
ATOM	3096	CA	ASN	426		-36.573	17,945	1.00	0.00	3A7
ATOM	3097	CB	ASN	426	0.515	-35.250	18.487	1.00	0.00	3A7
ATOM	3098	CG	ASN	426		-34.458	17.438	1.00	0.00	3A7
MOTA	3099	OD1	ASN	426		-34.963	16.848	1.00	0.00	3A7
ATOM	3100		ASN	426		-33.168	17.234	1.00	0.00	3A7
ATOM	3101	C	ASN	426	-	-36.329	16.915	1.00	0.00	. 3A7
ATOM	3102	0	ASN	426		-37.229	16.157	1.00	0.00	3A7 3A7
ATOM	3103	N	ILE	427		-35.090 -34.709	16.880 16.022	1.00	0.00	3A7
ATOM	3104 3105	CA CB	ILE	427 - 427		-33.632	16.647	1.00	0.00	3A7
ATOM ATOM	3106		ILE	427		-33.389	15.762	1.00	0.00	3A7
ATOM	3107		ILE	427		-34.009	18.097	1.00	0.00	3A7
ATOM	3108	CD	ILE	427		-35.302	18.218	1.00	0.00	3 <b>A</b> 7
MOTA	3109	C	ILE	427		-34.224	14.699	1.00	0.00	3A7
MOTA	3110	0	ILE	427	-2.782	-34.635	13.641	1.00	0.00	3A7
MOTA	3111	N	ASP	428		-33.326	14.741	1.00	0.00	3A7
MOTA	3112	CA	ASP	428		-32.752	13.555	1.00	0.00	3A7
MOTA	3113	СВ	ASP	428		-31.262	13.360	1.00	0.00	3A7
ATOM	3114	CG	ASP	428		-31.131	13.173	1.00	0.00	3A7
ATOM	3115		ASP	428		-31.683	12.169	1.00	0.00	3A7 3A7
ATOM	3116		ASP	428		-30.473 -32.877	14.030 13.650	1.00	0.00	3A7
ATOM ATOM	3117 3118	С 0	ASP ASP	428 428		-32.877	14.093	1.00	0.00	3A7
ATOM	3110	N	PRO	429		-34.003	13.251	1.00	0.00	3A7
ATOM	3120	CA	PRO	429		-34.177	13.157	1.00	0.00	3A7
ATOM	3121	CD	PRO	429		-35.245	12.998	1.00	0.00	3A7
ATOM	3122	СВ	PRO	429		-35.701	13.258	1.00	0.00	3A7
ATOM	3123	CG	PRO	429		-36.266	12.604	1.00	0.00	3A7
MOTA	3124	С	PRO	429	3.490	-33.658	11.858	1.00	0.00	3A7

ATOM	3125	0	PRO	429	2.892	-33.616	10.780	1.00	0.00	3A7
ATOM	3126	N	TYR	430		-33.325	11.967	1.00	0.00	3A7
ATOM	3127	CA	TYR	430		-33.153	10.884	1.00	0.00	3A7
ATOM	3128	СВ	TYR	430		-34.248	9.770	1.00	0.00	3A7
ATOM	3129	CG	TYR	430		-34.285	8.969	1.00	0.00	3A7
			TYR	430		-34.836	9.516	1.00	0.00	3A7
ATOM	3130					-33.566	7.779	1.00	0.00	3A7
ATOM	3131		TYR	430			8.926	1.00	0.00	3A7
ATOM	3132		TYR	430		-34.596	7.232	1.00	0.00	3A7
ATOM	3133		TYR	430		-33.267				3A7
MOTA	3134	CZ	TYR	430		-33.774	7.806	1.00	0.00	
ATOM	3135	ОН	TYR	430		-33.421	7.266	1.00	0.00	3A7
ATOM	3136	С	TYR	430		-31.761	10.274	1.00	0.00	3A7
ATOM	3137	0	TYR	430		-31.428	9.529	1.00	0.00	3A7
MOTA	3138	N	ILE	431	4.795	-30.877	10.599	1.00	0.00	3A7
ATOM	3139	ÇA	ILE	431	4.842	-29.502	10.146	1.00	0.00	3A7
ATOM	3140	CB	ILE	431	3.495	-28.893	9.784	1.00	0.00	3A7
ATOM	3141	CG2	ILE	431	2.954	-29.661	8.570	1.00	0.00	3A7
ATOM	3142	CG1	ILE	431	2.477	-28.800	10.949	1.00	0.00	3A7
ATOM	3143		ILE	431	1.966	-30.124	11.513	1.00	0.00	3A7
ATOM	3144	C	ILE	431	5.480	-28.630	11.193	1.00	0.00	3A7
ATOM	3145	ŏ	ILE	431		-27.509	10.893	1.00	0.00	3A7
ATOM	3146	N	TYR	432		-29.122	12.460	1.00	0.00	3A7
ATOM	3147	CA	TYR	432		-28.443	13.571	1.00	0.00	3A7
	3148	CB	TYR	432		-28.969	14.973	1.00	0.00	3A7
MOTA						-28.367	15.505	1.00	0.00	3A7
MOTA	3149	CG	TYR	432				1.00	0.00	3A7
MOTA	3150		TYR	432		-29.190	15.886			3A7
ATOM	3151		TYR	432		-27.004	15.799	1.00	0.00	
ATOM	3152		TYR	432		-28.665	16.575	1.00	0.00	3A7
MOTA	3153		TYR	432		-26.477	16.484	1.00	0.00	3A7
ATOM	3154	CZ	TYR	432		-27.307	16.878	1.00	0.00	3A7
MOTA	3155	ОН	TYR	432		-26.773	17.586	1.00	0.00	3A7
MOTA	3156	С	TYR	432		-28.741	13.531	1.00	0.00	3A7
MOTA	3157	0	TYR	432	8.161	-29.675	14.169	1.00	0.00	3A7
ATOM	3158	N	THR	433		-27.919	12.778	1.00	0.00	3A7
MOTA	3159	CA	THR	433	9.824	-28.119	12.506	1.00	0.00	3A7
ATOM	3160	СВ	THR	433	10.074	-28.167	10.995	1.00	0.00	3A7
ATOM	3161	OG1	THR	433	9.638	-26.980	10.336	1.00	0.00	3A7
ATOM	3162	CG2	THR	433	9.309	-29.368	10.401	1.00	0.00	3A7
ATOM	3163	С	THR	433		-27.070	13.107	1.00	0.00	3A7
MOTA	3164	0	THR	433	11.720	-26.744	12.459	1.00	0.00	3A7
ATOM	3165	N	PRO	434	10.544	-26.494	14.305	1.00	0.00	3A7
ATOM	3166	CA	PRO	434		-25.526	14.854	1.00	0.00	3A7
ATOM	3167	CD	PRO	434		-26.944	15.329	1.00	0.00	3A7
ATOM	3168	СВ	PRO	434		-25.003	16.098	1.00	0.00	3A7
ATOM	3169	CG	PRO	434		-26.220	16.622	1.00	0.00	3A7
ATOM	3170	c	PRO	434		-26.180	15.226	1.00	0.00	3A7
ATOM	3171	ŏ	PRO	434		-25.477	15.300	1.00	0.00	3A7
				435		-27.518	15.456	1.00	0.00	3A7
ATOM	3172	N	PHE			-28.253	15.844	1.00	0.00	3A7
ATOM	3173	CA	PHE	435	•	-29.173	17.045	1.00	0.00	3A7
ATOM	3174	CB	PHE	435				1.00	0.00	3A7
ATOM	3175	CG	PHE	435		-28.509	18.358	1.00	0.00	3A7
ATOM	3176		PHE	435		-27.557	18.520			3A7
ATOM	3177		PHE	435		-28.261	19.269	1.00	0.00	3A7 3A7
ATOM	3178		PHE	435		-26.403	19.460	1.00	0.00	
ATOM	3179		PHE	435		-27.600	20.460	1.00	0.00	3A7
ATOM	3180	CZ	PHE	435		-26.726	20.695	1.00	0.00	3A7
ATOM	3181	С	PHE	435		-29.099	14.689	1.00	0.00	3A7
MOTA	3182	0	PHE	435		-29.980	14.855	1.00	0.00	3A7
ATOM	3183	N	GLY	436		-28.834	13.469	1.00	0.00	3A7
MOTA	3184	CA	GLY	436		-29.495	12.269	1.00	0.00	3A7
MOTA	3185	C	GLY	436	13.733	-30.777	12.129	1.00	0.00	3A7
ATOM	3186	0	GLY	436	12.792	-31.061	12.870	1.00	0.00	3A7
ATOM	3187	N	SER	437	14.147	-31.599	11.152	1.00	0.00	3A7
ATOM	3188	CA	SER	437		-32.872	10.944	1.00	0.00	3A7
ATOM	3189	СВ	SER	437		-32.829	9.974	1.00	0.00	3A7
ATOM	3190	ŌĞ	SER	437		-32.079	10.518	1.00	0.00	3A7
ATOM	3191	c	SER	437		-33.730	10.351	1.00	0.00	3A7
ATOM	3192	ŏ	SER	437		-33.291	9.494	1.00	0.00	3A7
ATOM	3193	N	GLY	438		-35.006	10.788	1.00	0.00	3A7
ATOM	3194	CA	GLY	438		-36.010	10.184	1.00	0.00	3A7
ATOM	3195	C	GLY	438		-36.414	11.067	1.00	0.00	3A7
								1.00	0.00	3A7
MOTA	3196	0	GLY	438	10.326	-36.346	12.293	1.00	0.00	JAI

MOTA	3197	N	PRO	439	17.704 -	36.873	10.443	1.00	0.00	3A7
ATOM	3198	CA	PRO	439	18.897 -	37.275	11.180	1.00	0.00	3A7
MOTA	3199	CD	PRO	439	17.653 -		9.152	1.00	0.00	3A7
ATOM	3200	CB	PRO	439	19.741 -		10.170	1.00	0.00	3A7
MOTA	3201	CG	PRO	439	18.702 -		9.220	1.00	0.00 0.00	3A7 3A7
ATOM	3202 3203	C O	PRO PRO	439 439	19.700 <b>-</b> 20.523 -		11.729 12.614	1.00	0.00	3A7
ATOM ATOM	3203	N	ARG	440	19.490 -		11.217	1.00	0.00	3A7
ATOM	3205	CA	ARG	440	20.212 -		11.642	1.00	0.00	3A7
ATOM	3206	СВ	ARG	440	20.704 -		10.433	1.00	0.00	3A7
ATOM	3207	CG	ARG	440	21.775 -		9.617	1.00	0.00	3A7
ATOM	3208	CD	ARG	440	21.846 -	33.224	8.148	1.00	0.00	3A7
ATOM	3209	NE	ARG	440	20.618 -	33.741	7.458	1.00	0.00	3A7
ATOM	3210	CZ	ARG	440	20.391 -		6.123	1.00	0.00	3A7
ATOM	3211		ARG	440	19.299 -		5.537	1.00	0.00	3A7
ATOM	3212		ARG	440	21.244 -		5.371	1.00	0.00	3A7
ATOM	3213	C	ARG	440	19.307 -		12.480	1.00	0.00	3A7
ATOM	3214	0	ARG	440	19.471 -		12.565	1.00	0.00	3A7 3A7
ATOM	3215 3216	N	ASN	441 441	18.322 - 17.420 -		13.163 14.066	1.00	0.00	3A7
ATOM ATOM	3216	CA CB	ASN	441	16.263 -		14.515	1.00	0.00	3A7
ATOM	3218	CG	ASN	441	16.713 -		15.324	1.00	0.00	3A7
ATOM	3219		ASN	441	17.527 -		14.869	1.00	0.00	3A7
ATOM	3220		ASN	441	16.154 -		16.567	1.00	0.00	3A7
ATOM	3221	C	ASN	441	18.197 -		15.260	1.00	0.00	3A7
ATOM	3222	0	ASN	441	19.263 -	32.884	15.550	1.00	0.00	3A7
ATOM	3223	N	CYS	442	17.690 -	31.324	15.990	1.00	0.00	3A7
ATOM	3224	CA	CYS	442	18.409 -		17.097	1.00	0.00	3A7
ATOM	3225	СВ	CYS	442	17.629 -		17.676	1.00	0.00	3A7
ATOM	3226	SG	CYS	442	18.592 -		18.905	1.00	0.00	3A7 3A7
ATOM	3227	c	CYS	442	18.683 - 17.779 -		18.181 18.699	1.00	0.00	3A7
ATOM ATOM	3228 3229	о И	ILE	442 443	19.971 -		18.535	1.00	0.00	3A7
ATOM	3230	CA	ILE	443	20.405 -		19.531	1.00	0.00	3A7
ATOM	3231	СВ	ILE	443	21.872 -		19.324	1.00	0.00	3A7
ATOM	3232		ILE	443	22.414 ~		20.472	1.00	0.00	3A7
ATOM	3233		ILE	443	22.046 -		17.955	1.00	0.00	3A7
ATOM	3234	CD	ILE	443	21.378 -	35.291	17.849	1.00	0.00	3A7
ATOM	3235	С	ILE	443	20.167 -		20.902	1.00	0.00	3A7
ATOM	3236	0	ILE	443	20.008 -		21.894	1.00	0.00	3A7
ATOM	3237	N	GLY	444	20.106 -		20.975	1.00	0.00	3A7
ATOM	3238	CA	GLY	444	19.894 -		22.204	1.00	0.00	3A7 3A7
ATOM ATOM	3239 3240	C O	GLY GLY	444	18.471 - 18.222 -		22.535 23.479	1.00	0.00	3A7
ATOM	3241	N	MET	445	17.493 -		21.788	1.00	0.00	3A7
ATOM	3242	CA	MET	445	16.056 -		21.939	1.00	0.00	3A7
ATOM	3243	СВ	MET	445	15.279 -		21.002	1.00	0.00	3A7
ATOM	3244	CG	MET	445	13.742 -	31.222	21.137	1.00	0.00	3A7
MOTA	3245	SD	MET	. 445	12.898 -	32.098	19.780	1.00	0.00	3A7
MOTA	3246	CE	MET	445	13.584 -		20.107	1.00	0.00	3A7
MOTA		С	MET	445	15.558 -		23.349	1.00	0.00	3A7
ATOM	3248	0	MET	445	14.887 -		23.919	1.00	0.00	3A7
ATOM	3249	N	ARG	446	15.928 -		23.976	1.00	0.00	3A7
ATOM	3250	CA	ARG	446	15.476 - 15.826 -			1.00	0.00	3A7 3A7
MOTA MOTA	3251 3252	CB CG	ARG ARG	446 446	15.490 -		25.684 24.538	1.00	0.00	3A7
ATOM	3253	CD	ARG	446	15.588 -		24.911	1.00	0.00	3A7
ATOM	3254	NE	ARG	446	14.428 ~		25.799	1.00	0.00	3A7
ATOM	3255	CZ	ARG	446	14.005 -		25.986	1.00	0.00	3A7
ATOM	3256		ARG	446	12.921 -		26.780	1.00	0.00	3A7
ATOM	3257		ARG	446	14.658 <del>-</del>		25.394	1.00	0.00	3A7
MOTA	3258	С	ARG	446	16.001 -		26.348	1.00	0.00	3A7
ATOM	3259	0	ARG	446	15.276 -		27.248	1.00	0.00	3A7
ATOM	3260	N	PHE	447	17.267 -		26.201	1.00	0.00	3A7
ATOM	3261	CA	PHE	447	17.865 -		27.113	1.00	0.00	3A7
ATOM	3262	CB	PHE	447	19.408 -		27.061	1.00	0.00	3A7 3A7
ATOM ATOM	3263 3264	CG	PHE	447 447	19.952 - 20.810 -		26.613 25.520	1.00	0.00	3A7 3A7
ATOM	3265		PHE	447	19.433 -		27.086	1.00	0.00	3A7 3A7
ATOM	3266		PHE	447	20.971 -		24.778	1.00	0.00	3A7
ATOM	3267		PHE	447	19.526 -		26.291	1.00	0.00	3A7
ATOM	3268	CZ	PHE	447	20.229 -		25.096	1.00	0.00	3A7

MOTA	3269	С	PHE	447	17.285	-28.185	26.918	1.00	0.00	3A7
ATOM	3270	0	PHE	447	17.071	-27.458	27.881	1.00	0.00	3A7
ATOM	3271	N	ALA	448	16.949	-27.798	25.656	1.00	0.00	3A7
ATOM	3272	CA	ALA	448	16.406	-26.493	25.374	1.00	0.00	3A7
ATOM	3273	СВ	ALA	448	16.379	-26.216	23.882	1.00	0.00	3A7
MOTA	3274	С	ALA	448	15.020	-26.344	25.914	1.00	0.00	3A7
ATOM	3275	0	ALA	448	14.679	-25.313	26.493	1.00	0.00	3A7
ATOM	3276	N	LEU	449	14.197	-27.406	25.800	1.00	0.00	3A7
ATOM	3277	CA	LEU	449	12.842	-27.402	26.309	1.00	0.00	3A7
MOTA	3278	CB	LEU	449	12.029	-28.605	25.813	1.00	0.00	3A7
MOTA	3279	CG	LEU	449	11.639	-28.523	24.324	1.00	0.00	3A7
ATOM	3280		LEU	449	11.120	-29.879	23.807	1.00	0.00	3A7
MOTA	3281	CD2	LEU	449	10.621	-27.401	24.038	1.00	0.00	3A7
MOTA	3282	C	LEU	449		-27.422	27.811	1.00	0.00	3A7
ATOM	3283	0	LEU	449		-26.797	28.417	1.00	0.00	3A7
ATOM	3284	N	VAL	450		-28.111	28.454	1.00	0.00	3A7
ATOM	3285	CA	VAL	450		-28.171	29.893	1.00	0.00	3A7
ATOM	3286	CB	VAL	450		-29.213	30.345	1.00	0.00	3A7
ATOM	3287		VAL	450		-29.141	31.862	1.00	0.00	3A7
ATOM	3288		VAL	450		-30.592	30.049	1.00	0.00	3A7
ATOM	3289	C	VAL	450		-26.828	30.431	1.00	0.00	3A7
ATOM	3290	0	VAL	450		-26.345	31.364	1.00	0.00	3A7
ATOM	3291	N	ASN	451		-26.162	29.833	1.00	0.00	3A7
ATOM	3292	CA	ASN	451		-24.855	30.232	1.00	0.00	3A7
ATOM	3293	CB	ASN	451		-24.401	29.295	1.00	0.00	3A7
ATOM	3294	CG	ASN	451		-25.243	29.476	1.00	0.00	3A7
ATOM	3295		ASN	451		-26.089	30.369	1.00	0.00	3A7
ATOM ATOM	3296		ASN	451		-24.981	28.583	1.00	0.00	3A7
	3297 3298	C	ASN	451		-23.792	30.150	1.00	0.00	3A7
ATOM ATOM	3298	N N	ASN	451		-23.023	31.081	1.00	0.00	3A7
ATOM	3300	CA	MET MET	452 452		-23.759 -22.808	29.019	1.00	0.00	3A7
ATOM	3301	СВ	MET	452		-22.880	28.800 27.353	1.00	0.00	3A7
MOTA	3302	CG	MET	452		-22.090	26.370	1.00	0.00	3A7 3A7
ATOM	3303	SD	MET	452		-22.975	24.894	1.00	0.00	3A7
MOTA	3304	CE	MET	452		-23.810	24.359	1.00	0.00	3A7
ATOM	3305	c	MET	452		-22.982	29.778	1.00	0.00	3A7
ATOM	3306	ŏ	MET	452		-22.013	30.355	1.00	0.00	3A7
ATOM	3307	N	LYS	453		-24.236	30.042	1.00	0.00	3A7
MOTA	3308	CA	LYS	453		-24.536	30.965	1.00	0.00	3A7
ATOM	3309	СВ	LYS	453		-26.021	30.868	1.00	0.00	3A7
ATOM	3310	CG	LYS	453	8.486	-26.409	31.399	1.00	0.00	3A7
ATOM	3311	CD	LYS	453	8.218	-27.911	31.258	1.00	0.00	3A7
ATOM	3312	CE	LYS	453	8.280	-28.457	29.817	1.00	0.00	3A7
ATOM	3313	NZ	LYS	453	9.661	-28.675	29.322	1.00	0.00	. 3A7
MOTA	3314	С	LYS	453	10.616	-24.214	32.386	1.00	0.00	3A7
ATOM	3315	0	LYS	453	9.869	-23.577	33.112	1.00	0.00	3A7
ATOM	3316	N	LEU	454	11.836	-24.594	32.812	1.00	0.00	3A7
ATOM	3317	CA	LEU	454		-24.349	34.154	1.00	0.00	3A7
ATOM	3318	СВ	LEU	454	13.614		34.423	1.00	0.00	3A7
ATOM	3319	CG	LEU	454	13.420		34.462	1.00	0.00	3A7
ATOM	3320		LEU	454	14.712		34.874	1.00	0.00	3A7
ATOM	3321		LEU	454	.12.265		35.377	1.00	0.00	3A7
ATOM	3322	C	LEU	454	12.488		34.440	1.00	0.00	3A7
ATOM	3323	0	LEU	454	12.033		35.465	1.00	0.00	3A7
ATOM ATOM	3324	N	ALA	455	13.101		33.501	1.00	0.00	3A7
ATOM	3325	CA	ALA	455 455	13.303		33.621	1.00	0.00	3A7
MOTA	3326 3327	CB C	ALA	455	14.157 12.006		32.468	1.00	0.00	3A7
ATOM	3328	Ö	ALA ALA	455 455	11.803		33.668 34.569	1.00	0.00	3A7
ATOM	3329	N	LEU	456	11.065		32.730	1.00	0.00	3A7
ATOM	3330	CA	LEU	456		-19.468	32.730	1.00	0.00	3A7
ATOM	3331	СВ	LEU	456		-19.835	31.351	1.00	0.00	3A7 3A7
ATOM	3332	CG	LEU	456		-19.033	30.053	1.00	0.00	3A7 3A7
ATOM	3333	CD1		456	10.961		30.084	1.00	0.00	3A7 3A7
ATOM	3334	CD2		456		-20.054	28.836	1.00	0.00	3A7
ATOM	3335	C	LEU	456		-19.770	33.817	1.00	0.00	3A7
ATOM	3336	ŏ	LEU	456		-18.888	34.337	1.00	0.00	3A7
ATOM	3337	N	VAL	457		-21.025	34.323	1.00	0.00	3A7
ATOM	3338	CA	VAL	457		-21.445	35.499	1.00	0.00	3A7
ATOM	3339	СВ	VAL	457		-22.911	35.843	1.00	0.00	3A7
ATOM	3340	CG1		457		-23.325	37.263	1.00	0.00	3A7
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ATOM	3341	ÇG2	VAL	457	7.670	-23.765	34.841	1.00	0.00	3A7
MOTA	3342	С	VAL	457		-20.633	36.694	1.00	0.00	3A7
ATOM	3343	0	VAL	457		-20.161	37.444	1.00	0.00	3A7 3A7
ATOM	3344 3345	N CA	ARG ARG	458 458		-20.443 -19.722	36.892 38.015	1.00	0.00	3A7
ATOM ATOM	3346	CB	ARG	458		-19.996	38.164	1.00	0.00	3A7
ATOM	3347	CG	ARG	458		-21.369	38.758	1.00	0.00	3A7
ATOM	3348	CD	ARG	458	13.750	-21.581	38.977	1.00	0.00	3A7
MOTA	3349	NE	ARG	458		-21.751	37.641	1.00	0.00	3A7
MOTA	3350	CZ	ARG	458		-22.941	37.197	1.00	0.00	3A7 3A7
ATOM	3351	NH1		458 458		-22.979 -24.080	35.995 37.937	1.00	0.00	3A7
ATOM ATOM	3352 3353	NH2 C	ARG	458		-18.233	37.894	1.00	0.00	3A7
ATOM	3354	ŏ	ARG	458		-17.578	38.869	1.00	0.00	3A7
ATOM	3355	N	VAL	459	10.398	-17.640	36.691	1.00	0.00	3A7
MOTA	3356	CA	VAL	45 <del>9</del>		-16.217	36.448	1.00	0.00	3A7
MOTA	3357	СВ	VAL	459		-15.894	35.017	1.00	0.00	3A7
MOTA	3358	CG1		459		-14.508	34.526	1.00	0.00	3A7 3A7
ATOM	3359	CG2		459 459		-16.014 -15.789	34.950 36.752	1.00	0.00	3A7
ATOM ATOM	3360 3361	C 0	VAL	459		-14.855	37.511	1.00	0.00	3A7
ATOM	3362	N	LEU	460		-16.538	36.226	1.00	0.00	3A7
ATOM	3363	CA	LEU	460	6.397	-16.237	36.374	1.00	0.00	3A7
ATOM	3364	CB	LEU	460		-17.011	35.340	1.00	0.00	3A7
MOTA	3365	CG	LEU	460		-16.588	33.893	1.00	0.00	3A7
ATOM	3366	CD1		460		-17.596	32.898 33.610	1.00	0.00	3A7 3A7
ATOM ATOM	3367 3368	CD2 C	LEU	460 460		-15.150 -16.582	37.736	1.00	0.00	3A7
ATOM	3369	o	LEU	460		-16.068	38.141	1.00	0.00	3A7
ATOM	3370	N	GLN .	461		-17.449	38.498	1.00	0.00	3A7
ATOM	3371	CA	GLN	461	6.249	-17.756	39.877	1.00	0.00	3A7
ATOM	3372	CB	GLN	461		-19.025	40.414	1.00	0.00	3A7
ATOM	3373	CG	GLN	461		-19.729	41.554	1.00	0.00 0.00	3A7 3A7
MOTA	3374 3375	CD	GLN GLN	461 461		-21.033 -21.463	41.909 41.220	1.00	0.00	3A7
MOTA MOTA	3376		GLN	461		-21.670	43.029	1.00	0.00	3A7
ATOM	3377	C	GLN	461		-16.632	40.808	1.00	0.00	3A7
ATOM	3378	0	GLN	461	5.945	-16.385	41.809	1.00	0.00	3A7
ATOM	3379	N	ASN	462		-15.950	40.487	1.00	0.00	3A7
ATOM	3380	CA	ASN	462		-15.014	41.373	1.00	0.00	3A7 3A7
ATOM	3381	CB	ASN	462 462		-15.166 -16.436	41.353	1.00	0.00	3A7
MOTA MOTA	3382 3383	CG OD1	ASN ASN	462		-17.563	41.666	1.00	0.00	3A7
ATOM	3384		ASN	462		-16.227	43.317		0.00	3A7
ATOM	3385	C -	ASN	462	8.026	-13.582	41.041	1.00	0.00	3A7
ATOM	3386	0	ASN	462		-12.710	41.888	1.00	0.00	3A7
ATOM	3387	N	PHE	463		-13.284	39.807	1.00	0.00	3A7 3A7
MOTA	3388	CA	PHE	463		-11.906 -11.416	39.372 38.535	1.00	0.00	3A7
ATOM ATOM	3389 3390	CB CG	PHE PHE	463 463		-11.416	39.308	1.00	0.00	3A7
ATOM	3391		PHE	463		-12.474	38.996	1.00	0.00	3A7
ATOM	3392		PHE	463		-10.594	40.340	1.00	0.00	3A7
ATOM	3393	CE1	PHE	463	12.021	-12.568	39.714	1.00	0.00	3A7
MOTA	3394		PHE	463			41.057			3A7
ATOM	3395	CZ	PHE	463		-11.673	40.747 38.530	1.00	0.00	3A7 3A7
ATOM TOM	3396 3397	С 0	PHE PHE	463 463		-11.715 -12.637	37.862	1.00	0.00	3A7
ATOM	3398	N	SER	464		-10.452	38.530	1.00	0.00	3A7
MOTA	3399	CA	SER	464	4.607		37.639	1.00	0.00	3A7
MOTA	3400	СВ	SER	464	3.437		38.330	1.00	0.00	3A7
MOTA	3401	OG	SER	464	3.854		39.167	1.00	0.00	3A7
ATOM	3402	C	SER	464	5.295		36.654	1.00	0.00	3A7 3A7
ATOM	3403	N O	SER Phe	464 465	5.987 5.122		37.035 35.343	1.00	0.00	3A7
ATOM ATOM	3404 3405	N CA	PHE	465	5.823		34.275	1.00	0.00	3A7
ATOM	3406	CB	PHE	465	6.320		33.195	1.00	0.00	3A7
ATOM	3407	CG	PHE	465	7.476	-10.312	33.835	1.00	0.00	3A7
ATOM	3408		PHE	465		-11.547	34.451	1.00	0.00	3A7
MOTA	3409		PHE	465	8.689		33.959	1.00	0.00	3A7
ATOM	3410		PHE	465		-12.080	35.204	1.00	0.00	3A7 3A7
ATOM	3411 3412	CE2	PHE PHE	465 465		-10.176 -11.399	34.692 35.322	1.00	0.00	3A7
ATOM	7416	C4	FUE	303	2.304	.1.333	,	1.00	3.23	

ATOM	3413	С	PHE	465	4.919	-7.687	33.592	1.00	0.00	3A7
ATOM	3414	ō	PHE	465	3.724	-7.936	33.425	1.00	0.00	3A7
ATOM	3415	N	LYS	466	5.493	-6.560	33.115	1.00	0.00	3A7
ATOM	3416	CA	LYS	466	4.734	-5.582	32.382	1.00	0.00	3A7
ATOM	3417	СВ	LYS	466	4.290	-4.427	33.296	1.00	0.00	3A7
ATOM	3418	CG	LYS	466	3.397	-4.837	34.480	1.00	0.00	3A7
ATOM	3419	CD	LYS	466	2.972	-3.643	35.348	1.00	0.00	3A7
			LYS	466	2.140	-4.046	36.574	1.00	0.00	3A7
MOTA	3420	CE			2.919	-4.922	37.481	1.00	0.00	3A7
ATOM	3421	NZ	LYS	466		-5.043	31.290	1.00	0.00	3A7
ATOM	3422	C	LYS	466	5.602		31.526	1.00	0.00	3A7
ATOM	3423	0	LYS	466	6.771	-4.756	30.080	1.00	0.00	3A7
MOTA	3424	N	PRO	467	5.061	-4.811		1.00	0.00	3A7
MOTA	3425	CA	PRO	467	5.708	-4.063	29.024		0.00	3A7
ATOM	3426	CD	PRO	467	3.897	-5.529	29.577	1.00		3A7 3A7
ATOM	3427	СВ	PRO	467	4.867	-4.318	27.759.		0.00	3A7
MOTA	3428	CG	PRO	467	4.104	-5.604	28.064	1.00	0.00	
ATOM	3429	С	PRO	467	5.709	-2.585	29.358	1.00	0.00	3A7
ATOM	3430	O <sub>.</sub>	PRO	467	4.657	-2.040	29.696	1.00	0.00	3A7
MOTA	3431	N	CYS	468	6.875	-1.912	29.284	1.00	0.00	3A7
ATOM	3432	CA	CYS	468	7.012	-0.524	29.684	1.00	0.00	3A7
ATOM	3433	СВ	CYS	468	8.466	-0.147	30.062	1.00	0.00	3A7
ATOM	3434	SG	CYS	468	9.057	-1.091	31.487	1.00	0.00	3A7
ATOM	3435	С	CYS	468	6.616	0.383	28.544	1.00	0.00	3A7
ATOM	3436	0	CYS	468	6.411	1.583	28.713	1.00	0.00	3 <b>A</b> 7
ATOM	3437	N	LYS	469	6.540	-0.205	27.334	1.00	0.00	· 3A7
ATOM	3438	CA	LYS	469	6.355	0.499	26.104	1.00	0.00	3A7
ATOM	3439	СВ	LYS	469	7.640	0.501	25.281	1.00	0.00	3A7
ATOM	3440	CG	LYS	469	8.757	1.350	25.918	1.00	0.00	3A7
ATOM	3441	CD	LYS	469	10.000	1.530	25.028	1.00	0.00	3A7
ATOM	3442	CE	LYS	469	9.788	2.435	23.807	1.00	0.00	3A7
ATOM	3443	NZ	LYS	469	9.393	3.802	24.218	1.00	0.00	3A7
ATOM	3444	С	LYS	469	5.347	-0.291	25.354	1.00	0.00	3A7
ATOM	3445	0	LYS	469	5.575	-1.459	25.050	1.00	0.00	3A7
ATOM	3446	N	GLU	470	4.138	0.226	25.134	1.00	0.00	3A7
ATOM	3447	CA	GLU	470	3.141	-0.604	24.504	1.00	0.00	3A7
ATOM	3448	СВ	GLU	470	1.701	-0.299	24.997	1.00	0.00	3A7
ATOM	3449	CG	GLU	470	1.488	-0.619	26.491	1.00	0.00	3A7
ATOM	3450	CD	GLU	470	1.553	-2.121	26.773	1.00	0.00	3A7
ATOM	3451		GLU	470	1.559	-2.928	25.806	1.00	0.00	3A7
ATOM	3452		GLU	470	1.584	-2.480	27.981	1.00	0.00	3A7
ATOM	3453	C	GLU	470	3.348	-0.317	23.071	1.00	0.00	3A7
ATOM	3454	ŏ	GLU	470	4.315	-0.740	22.429	1.00	0.00	3A7
MOTA	3455	N	THR	471	2.368	0.501	22.575	1.00	0.00	3A7
ATOM	3456	CA	THR	471	2.160	1.284	21.360	1.00	0.00	3A7
MOTA	3457	СВ	THR	471	2.447	2.764	21.659	1.00	0.00	3A7
ATOM	3458		THR	471	1.929	3.641	20.661	1.00	0.00	3A7
ATOM	3459		THR	471	3.946	3.049	21.904	1.00	0.00	3A7
ATOM	3460	C	THR	471	2.841	0.808	20.088	1.00	0.00	3A7 .
	3461	ò	THR	471	3.308	1.608	19.278	1.00	0.00	3A7
ATOM ATOM	3462	N	GLN	472	2.875	-0.535		1.00	0.00	3A7
	3463	CA	GLN	472	3.410	-1.235	18.731	1.00	0.00	3A7
ATOM ATOM	3464	СВ	GLN	472	2.623	-0.915	17.428	1.00	0.00	3A7
	3465	CG	GLN	472	2.830	-1.913	16.270	1.00	0.00	3A7
ATOM	3466				2.412				0.00	3A7
ATOM		CD	GLN	472 472	3.252	-4.222	16.818	1.00	0.00	3A7
ATOM	3467		GLN		1.077	-3.502	16.944	1.00	0.00	3A7
ATOM	3468		GLN	472	4.893	-0.974	18.547	1.00	0.00	3A7
ATOM	3469	C	GLN	472	5.362	-0.673	17.450	1.00	0.00	3A7
ATOM	3470	0	GLN	472		-1.090	19.658	1.00	0.00	3A7
ATOM	3471	N	ILE	473	5.672		19.613	1.00	0.00	3A7
MOTA	3472	CA	ILE	473	7.130	-0.993				3A7
MOTA	3473	CB	ILE	473	7.790	-0.303	20.808	1.00	0.00	3A7
ATOM	3474		ILE	473	9.304	-0.020	20.648	1.00		3A7
ATOM	3475		ILE	473	7.030	1.009	21.146	1.00	0.00	3A7
MOTA	3476	CD	ILE	473	7.180	2.124	20.104	1.00	0.00	3A7
MOTA	3477	C	ILE	473	7.840	-2.153	19.174	1.00	0.00	
ATOM	3478	0	ILE	473	8.886	-1.850	18.619	1.00	0.00	3A7
MOTA	3479	N	PRO	474	7.388	-3.403	19.312	1.00	0.00	3A7
MOTA	3480	CA	PRO	474	8.307	-4.483	19.289	1.00	0.00	3A7
ATOM	3481	CD	PRO	474	6.293	-3.751	20.216	1.00	0.00	3A7
MOTA	3482	CB	PRO	474	7.554	-5.688	19.660	1.00	0.00	3A7
ATOM	3483	CG	PRO	474	6.580	-5.162	20.707	1.00	0.00	3A7
MOTA	3484	С	PRO	474	9.042	-4.735	18.043	1.00	0.00	3A7

ATOM	3485	0	PRO	474	8.461	-4.845	16.967	1.00	0.00	3A7
ATOM	3486	N	LEU	475	10.363	-4.780	18.250	1.00	0.00	3A7
ATOM	3487	CA	LEU	475	11.281	-4.868	17.212	1.00	0.00	3A7
ATOM	3488	СВ	LEU	475	12.494	-3.929	17.438	1.00	0.00	3A7
ATOM	3489	CG	LEU	475	12.127	-2.431	17.558	1.00	0.00	3A7
ATOM	3490	CD1		475	13.371	-1.592	17.906	1.00	0.00	3A7
ATOM	3491	CD2		475	11.432	-1.891	16.293	1.00	0.00	3A7
ATOM	3492	С	LEU	475	11.786	-6.229	17.109	1.00	0.00	3A7
ATOM	3493	ō	LEU	475	12.315	-6.781	18.064	1.00	0.00	3A7
ATOM	3494	N	LYS	476	11.627	-6.792	15.915	1.00	0.00	3A7
ATOM	3495	CA	LYS	476	12.112	-8.088	15.588	1.00	0.00	3A7
ATOM	3496	CB	LYS	476	11.115	-8.801	14.712	1.00	0.00	3A7
ATOM	3497	CG	LYS	476	9.772	-9.009	15.441	1.00	0.00	3A7
ATOM	3498	CD	LYS	476	8.674	-9.612	14.555	1.00	0.00	3A7
MOTA	3499	CE	LYS	476	8.939	-11.068	14.167	1.00	0.00	3A7
ATOM	3500	NZ	LYS	476	7.894	-11.545	13.235	1.00	0.00	3A7
ATOM	3501	С	LYS	476	13.325	-7.870	14.776	1.00	0.00	3A7
ATOM	3502	0	LYS	476	13.337	-7.042	13.874	1.00	0.00	3A7
ATOM	3503	N	LEU	477	14.395	-8.621	15.042	1.00	0.00	3A7
ATOM	3504	CA	LEU	477	15.554	-8.551	14.210	1.00	0.00	3A7
ATOM	3505	CB	LEU	477	16.856	-8.930	14.889	1.00	0.00	3A7
MOTA	3506	CG	LEU	477	18.083	-8.017	14.617	1.00	0.00	3A7
ATOM	3507	CD1	LEU	477	19.159	-8.239	15.698	1.00	0.00	3A7
ATOM	3508	CD2	LEU	477	18.705	-8.182	13.223	1.00	0.00	3A7
MOTA	3509	С	LEU	477	15.422	-9.412	13.099	1.00	0.00	3A7
MOTA	3510	0	LEU	477	14.926		13,208	1.00	0.00	3A7
ATOM	3511	N	ARG	478	15.810	-8.885	11.967	1.00	0.00	3A7
ATOM	3512	CA	ARG	478	15.460	-9.604	10.853	1.00	0.00	3A7
MOTA	3513	CB	ARG	478	14.781	-8.647	9.829	1.00	0.00	3A7
MOTA	3514	CG	ARG	478	13.512	-7.955	10.358	1.00	0.00	3A7
MOTA	3515	CD	ARG	478	12.226	-8.561	9.784	1.00	0.00	3A7 3A7
MOTA	3516	NE	ARG	478	12.180		10.198	1.00	0.00	3A7
MOTA	3517	CZ	ARG	478		-10.528	10.977	1.00	0.00	3A7
ATOM	3518		ARG	478		-11.836	11.366	1.00	0.00	3A7
ATOM	3519		ARG	478	10.121	-9.764	11.352	1.00	0.00	3A7
ATOM	3520	С	ARG	478		-10.335	10.080	1.00	0.00	3A7
ATOM	3521	0	ARG	478		-10.652	8.927 10.632	1.00	0.00	3A7
ATOM	3522	N	PHE	479		-10.610 -10.706	9.806	1.00	0.00	3A7
ATOM	3523	CA	PHE	479		-10.235	10.539	1.00	0.00	3A7
ATOM	3524	CB	PHE	479	21.147	-9.680	9.633	1.00	0.00	3A7
ATOM	3525	CG	PHE	479 479	20.917	-8.497	8.929	1.00	0.00	3A7
ATOM	3526		PHE	479		-10.322	9.495	1.00	0.00	3A7
MOTA	3527 3528		PHE	479	21.894	-7.970	8.093	1.00	0.00	3A7
MOTA MOTA	3529		PHE	479		-9.799	8.652	1.00	0.00	3A7
ATOM	3530	CZ	PHE	479	23.115	-8.622	7.951	1.00	0.00	3A7
MOTA	3531	c	PHE	479		-12.054	9.251	1.00	0.00	3A7
ATOM	3532	ō	PHE	479		-12.120	8.413	1.00	0.00	3A7
MOTA	3533	N	GLY	480		-13.153	9.632	1.00	0.00	3A7
ATOM	3534	CA	GLY	480		-14.416	8.969	1.00	0.00	3A7
ATOM	3535	C	GLY	480		-15.080	9.499	1.00	0.00	3A7
ATOM	3536	ō	GLY	480		-14.455	9.781	1.00	0.00	3A7
ATOM	3537	N	GLY	481	19.874	-16.400	9.691	1.00	0.00	3A7
ATOM	3538	CA	GLY	481	20.747	-17.199	10.480	1.00	0.00	3A7
ATOM	3539	С	GLY	481	19.999	-17.404	11.756	1.00	0.00	3A7
ATOM	3540	0	GLY	481		-18.530	12.126	1.00	0.00	3A7
MOTA	3541	N	LEU	482		-16.297	12.465	1.00	0.00	3A7
ATOM	3542	CA	LEU	482	19.157	-16.393	13.801	1.00	0.00	. 3A7
MOTA	3543	CB	LEU	482		-16.416	14.840	1.00	0.00	3A7
MOTA	3544	CG	LEU	482		-17.132	16.175	1.00	0.00	3A7
ATOM	3545	CD1	LEU	482		-16.443	17.020	1.00	0.00	3A7
ATOM	3546		LEU	482		-18.634	15.963	1.00	0.00	3A7
ATOM	3547	С	LEU	482		-15.192	13.998	1.00	0.00	3A7
ATOM	3548	0	LEU	482		-14.069	13.996	1.00	0.00	3A7 3A7
ATOM	3549	N	LEU	483		-15.412	14.210	1.00	0.00	3A7
MOTA	3550	CA	LEU	483		-14.371	14.462	1.00	0.00	3A7
ATOM	3551	СВ	LEU	483		-14.799	14.069	1.00	0.00	3A7
MOTA	3552	CG	LEU	483		-14.905	12.543	1.00	0.00	3A7
ATOM	3553		LEU	483		-15.253	12.231	1.00 1.00	0.00	3A7
MOTA	3554		LEU	483		-13.634	11.775	1.00	0.00	3A7
MOTA	3555	C	LEU	483		-14.055	15.923	1.00	0.00	3A7
ATOM	3556	0	LEU	483	13./99	-14.926	16.767	1.00	0.00	<b></b>

ATOM	3557	N	LEU	484	16.246 -	12.778	16.236	1.00	0.00	3A7
ATOM	3558	CA	LEU	484	16.374 -		17.588	1.00	0.00	3A7
ATOM	3559	СВ	LEU	484	17.753 -		17.812	1.00	0.00	3A7
ATOM	3560	CG	LEU	484	18.984 -		17.710	1.00	0.00	3A7
ATOM	3561		LEU	484	20.271 -		17.445	1.00	0.00	3A7
ATOM	3562		LEU	484	19.140 -	•	18.970	1.00	0.00	3A7
ATOM	3563	C	LEU	484	15.345 -		17.861	1.00	0.00	3A7
ATOM	3564	ō	LEU	484	14.779 -		16.981	1.00	0.00	3A7
ATOM	3565	N	THR	485	15.149 -		19.142	1.00	0.00	3A7
ATOM	3566	CA	THR	485	14.449	-9.702	19.526	1.00	0.00	3A7
ATOM	3567	СВ	THR	485	13.528	-9.902	20.697	1.00	0.00	3A7
ATOM	3568	0G1	THR	485	12.643 -	-10.981	20.430	1.00	0.00	3A7
ATOM	3569	CG2	THR	485	12.694	-8.634	20.978	1.00	0.00	3A7
ATOM	3570	С	THR	485	15.542	-8.739	19.870	1.00	0.00	3A7
ATOM	3571	0	THR	485	16.525	-9.095	20.514	1.00	0.00	3A7
ATOM	3572	N	GLU	486	15.407	-7.491	19.395	1.00	0.00	3A7 3A7
ATOM	3573	CA	GLU	486	16.478	-6.537	19.402	1.00	0.00	3A7 3A7
ATOM	3574	CB	GLU	486	16.229	-5.476	18.329	1.00	0.00	3A7
ATOM	3575	CG	GLU	486	16.097	-6.056	16.918	1.00	0.00	3A7
ATOM	3576	CD	GLU	486	16.045	-4.920	15.900	1.00	0.00	3A7
ATOM	3577		GLU	486	15.044	-4.847	15.140 15.863	1.00	0.00	3A7
ATOM	3578		GLU	486	17.014	-4.115 -5.904	20.729	1.00	0.00	3A7
ATOM	3579	С	GLU	486	16.763 17.821	-6.121	21.297	1.00	0.00	3A7
ATOM	3580	0	GLU	486	15.871	-5.074	21.275	1.00	0.00	3A7
ATOM	3581	N	LYS	487	16.181	-4.394	22.523	1.00	0.00	3A7
MOTA	3582	CA	LYS	487 487	16.681	-2.935	22.345	1.00	0.00	3A7
MOTA	3583	CB	LYS LYS	487	18.078	-2.831	21.710	1.00	0.00	3A7
ATOM	3584 3585	CG CD	LYS	487	18.582	-1.386	21.553	1.00	0.00	3A7
MOTA MOTA	3586	CE	LYS	487	17.737	-0.521	20.606	1.00	0.00	3A7
MOTA	3587	NZ	LYS	487	17.683	-1.111	19.249	1.00	0.00	3A7
ATOM	3588	c	LYS	487	14.847	-4.380	23.208	1.00	0.00	3A7
ATOM	3589	ŏ	LYS	487	14.110	-3.436	22.965	1.00	0.00	3A7
ATOM	3590	N	PRO	488	14.469	-5.369	24.036	1.00	0.00	3A7
ATOM	3591	CA	PRO	488	13.160	-5.418	24.666	1.00	0.00	3A7
ATOM	3592	CD		. 488	15.099	-6.687	23.995	1.00	0.00	3A7
ATOM	3593	СВ	PRO	488	12.772	-6.900	24.541	1.00	0.00	3A7
ATOM	3594	CG	PRO	488	14.103	-7.653	24.646	1.00	0.00	3A7
MOTA	3595	С	PRO	488	13.285	-4.931	26.063	1.00	0.00	3A7
ATOM	3596	0	PRO	488	14.207	-5.350	26.760	1.00	0.00	3A7 3A7
ATOM	3597	N	ILE	489	12.369	-4.042	26.506	1.00	0.00	3A7
MOTA	3598	CA	ILE	489	12.431	-3.564	27.858	1.00 1.00	0.00 0.00	3A7
ATOM	3599	СВ	ILE	489	12.824	-2.096	28.021 27.475	1.00	0.00	3A7
ATOM	3600		ILE	489	14.258 11.831	-1.923 -1.092	27.392	1.00	0.00	3A7
MOTA	3601		ILE	489 489	12.182	0.356	27.747	1.00	0.00	3A7
ATOM	3602	CD	ILE	489	11.136	-3.837	28.577	1.00	0.00	- 3A7
ATOM	3603	0	ILE	489	10.052	-3.733	28.009	1.00	0.00	3A7
ATOM ATOM	3604 3605	N .	VAL	490	11.230	-4.209	29.878	1.00	0.00	. 3A7
MOTA	3606	CA	VAL	490	10.101	-4.648	30.674	1.00	0.00	3A7
ATOM	3607	СВ	VAL	490	9.925	-6.155	30.572	1.00	0.00	3A7
ATOM	3608		VAL	490	9.245	-6.911	31.734	1.00	0.00	3A7
ATOM	3609		VAL	490	9.143	-6.483	29.279	1.00	0.00	3A7
ATOM	3610	С	VAL	490	10.398	-4.303	32.085	1.00	0.00	3A7
MOTA	3611	0	VAL	490	11.537	-4.064	32.455	1.00	0.00	3A /
MOTA	3612	N	LEU	491	9.344	-4.289	32.927	1.00	0.00	3A7
MOTA	3613	CA	LEU	491	9.438	-4.005	34.328	1.00	0.00	3A7 3A7
MOTA	3614	CB	LEU	491	8.379	-2.956	34.702	1.00	0.00	3A7
MOTA	3615	CG	LEU	491	8.991	-1.575	35.041	1.00	0.00	3A7
ATOM	3616		LEU	491	7.898	-0.495	35.142	1.00	0.00	3A7
ATOM	3617		LEU	491	9.848	-1.615	36.322	1.00	0.00	3A7
ATOM	3618	C	LEU	491	9.183	-5.273	35.064 34.680	1.00	0.00	3A7
ATOM	3619	0	LEU	491	8.303	-6.043 -5.530	36.165	1.00	0.00	3A7
MOTA	3620	N	LYS	492	9.934 9.855	-6.761	36.930	1.00	0.00	3A7
ATOM	3621	CA	LYS	492 492	11.254	-7.391	37.203		0.00	3A7
ATOM	3622	CB	LYS LYS		12.184	-6.661	38.201	1.00	0.00	3A7
ATOM ATOM	3623 3624	CG CD	LYS	492	12.735	-5.301	37.743			3A7
ATOM	3625	CE	LYS		12.568	-4.191	38.784			3A7
ATOM	3626	NZ	LYS		11.143	-3.831	38.925			3A7
MOTA	3627	C	LYS		9.148	-6.537	38.247			3A7
ATOM	3628		LYS		9.344	-7.295	39.196			` 3A7

ATOM	3629	N	ALA	493	8.315	-5.466	38.338	1.00	0.00	3A7
ATOM	3630	CA	ALA	493	7.783	-4.923	39.576	1.00	0.00	3A7
ATOM	3631	CB	ALA	493	7.164	-3.529	39.347	1.00	0.00	3A7
ATOM	3632	С	ALA	493	6.735	-5.798	40.223	1.00	0.00	3A7
ATOM	3633	0	ALA	493	5.607	-5.896	39.745	1.00	0.00	3A7
ATOM	3634	N	GLU	494	7.121	-6.449	41.348	1.00	0.00	3A7
ATOM	3635	CA	GLU	494	6.270	-7.353	42.081	1.00	0.00	3A7 3A7
ATOM	3636	CB	GLU	494	6.221	-8.771	41.447	1.00	0.00	3A7
ATOM	3637	CG	GLU	494	5.073	-9.691	41.921 43.282	1.00	0.00	3A7
ATOM	3638	CD	GLU	494 494		-10.327 -10.984	43.425	1.00	0.00	3A7
ATOM	3639	OE1		494		-10.334	44.193	1.00	0.00	3A7
ATOM	3640 3641	OE2	GLU	494	6.833	-7.451	43.468	1.00	0.00	3A7
ATOM ATOM	3642	Ö	GLU	494	6.097	-7.692	44.424	1.00	0.00	3A7
MOTA	3643	N	SER	495	8.180	-7.291	43.592	1.00	0.00	3A7
ATOM	3644	ÇA	SER	495	9.005	-7.634	44.741	1.00	0.00	3A7
ATOM	3645	СВ	SER	495	10.488	-7.267	44.500	1.00	0.00	3A7
MOTA	3646	OG	SER	495	10.963	-7.890	43.315	1.00	0.00	3A7
ATOM	3647	С	SER	495	8.584	-6.990	46.046	1.00	0.00	3A7
ATOM	3648	0	SER	495	8.318	-5.791	46.117	1.00	0.00	3A7
MOTA	3649	N	ARG	496	8.506	-7.831	47.102	1.00	0.00	3A7
MOTA	3650	CA	ARG	496	8.050	-7.468	48.419	1.00	0.00	3A7
ATOM	3651	CB	ARG	496	6.781	-8.270	48.810	1.00	0.00	3A7 3A7
MOTA	3652	CG	ARG	496	6.173	-7.918	50.178	1.00	0.00	3A7
MOTA	3653	CD	ARG	496	4.896	-8.715	50.471	1.00	0.00	3A7
ATOM	3654	NE	ARG	496	4.413	-8.345	51.841	1.00	0.00	3A7
MOTA	3655	CZ	ARG	496	3.354	-8.981 -8.609	52.430 53.681	1.00	0.00	3A7
ATOM	3656		ARG	496 496	2.955 2.696	-9.982	51.778	1.00	0.00	3A7
ATOM ATOM	3657 3658	C	ARG	496	9.179	-7.785	49.356	1.00	0.00	3A7
ATOM	3659	Ö	ARG	496	9.927	-8.738	49.139	1.00	0.00	3A7
ATOM	3660	N	ASP	497	9.312	-6.984	50.445	1.00	0.00	3A7
ATOM	3661	CA	ASP	497	10.298	-7.171	51.489	1.00	0.00	3A7
ATOM	3662	СВ	ASP	497	10.821	-5.830	52.089	1.00	0.00	,3A7
ATOM	3663	CG ·	ASP	497	9.707	-4.881	52.551	1.00	0.00	3A7
MOTA	3664	OD1	λSP	497	8.940	-4.387	51.682	1.00	0.00	3A7
MOTA	3665	OD2	ASP	497	9.625	-4.629	53.783	1.00	0.00	3A7
ATOM	3666	С	ASP	497	9.711	-8.068	52.560	1.00	0.00	3A7
MOTA	3667	0	ASP	497	8.985	-7.622	53.447	1.00	0.00	3A7 3A7
ATOM	3668	N	GLU	498	10.021	-9.384	52.458	1.00	0.00 0.00	3A7
MOTA	3669	CA	GLU	498		-10.423	53.314	1.00	0.00	3A7
MOTA	3670	CB	GLU	498		-11.610 -11.185	52.501 51.557	1.00	0.00	3A7
ATOM	3671	CG	GLU	498 498		-12.413	50.822	1.00	0.00	3A7
ATOM	3672 3673	CD OE1	GLU	498		-12.728	50.989	1.00	0.00	3A7
ATOM ATOM	3674	OE2	GLU	498		-13.049	50.081	1.00	0.00	3A7
MOTA	3675	C	GLU	498		-10.918	54.195	1.00	0.00	3A7
ATOM	3676	ō	GLU	498		-10.403	54.157	1.00	0.00	3A7
ATOM	3677	N	THR	499		-11.961	55.010	1.00	0.00	3A7
ATOM	3678	CA	THR	499	11.248	-12.606	55.905	1.00	0.00	3A7
ATOM	3679	СВ	THR	499		-12.970	57.245	1.00	0.00	3A7
ATOM	3680	OG1	THR	499		-13.726	57.084	1.00	0.00	3A7
ATOM	3681	CG2	THR	499		-11.664	57.998	1.00	0.00	3A7
MOTA	3682	С	THR	499		-13.836	55.217	1.00	0.00	3A7 3A7
MOTA	3683	0	THR	499		-14.244	54.163	1.00	0.00	3A7
MOTA	3684	N	VAL	500		-14.455	55.826 55.300	1.00	0.00	3A7
MOTA	3685	CA	VAL	500		-15.621 -15.588	55.594	1.00	0.00	3A7
MOTA	3686	CB	VAL VAL	500 500		-15.508	57.109	1.00	0.00	3A7
MOTA MOTA	3687 3688		VAL	500		-16.768	54.903	1.00	0.00	3A7
ATOM	3689	C	VAL	500		-16.864	55.847	1.00	0.00	3A7
ATOM	3690	Ö	VAL	500		-16.984	57.047	1.00	0.00	3A7
ATOM	3691	N	SER	501		-17.816	54.939	1.00	0.00	3A7
ATOM	3692	CA	SER	501		-19.059	55.286	1.00	0.00	3A7
ATOM	3693	СВ	SER	501		-18.950	55.320	1.00	0.00	3A7
ATOM	3694	OG	SER	501		-20.142	55.806		0.00	3A7
MOTA	3695	С	SER	501		-20.035	54.235	1.00	0.00	3A7
ATOM	3696	0	SER	501		-21.094	54.550	1.00	0.00	3A7
MOTA	3697	N	GLY	502		-19.677	52.947	1.00	0.00	3A7 3A7
ATOM	3698	CA	GLY	502		-20.464	51.805			3A7 3A7
MOTA	3699	C	GLY	502		-19.693	51.074	1.00		3A7
ATOM .	3700	0	GLY	502	13.335	-18.585	50.602	1.00	0:00	JAI

ATOM	3701	N	ALA	503	14.804	-20.283	50.980	1.00	0.00	3A7
ATOM	3702	CA	ALA	503	15.970	-19.715	50.338	1.00	0.00	3A7
ATOM	3703	СВ	ALA	503	15.775	-19.401	48.838	1.00	0.00	3A7
ATOM	3704	С	ALA	503	16.423	-18.443	51.073	1.00	0.00	3A7
ATOM	3705	OT1	ALA	503	17.016	-18.589	52.175	1.00	0.00	3A7
ATOM	3706	OT2	ALA	503	16.167	-17.323	50.557	1.00	0.00	3A7
TER	3707		ALA	503						
HETATM		FE	HEM	600	19.802	-26.909	18.195	1.00	0.00	HEM
HETATM		NA	HEM	600		-26.973	16.343	1.00	0.00	HEM
HETATM		NB	HEM	600		-25.763	18.746	1.00	0.00	HEM
HETATM		NC	HEM	600		-26.830	20.017	1.00	0.00	HEM
HETATM		ND	HEM	600		-28.034	17.616	1.00	0.00	HEM
HETATM		ClA		600		-27.653	15.248	1.00	0.00	HEM
HETATM		C2A		600		-27.461	14.072	1.00	0.00	HEM
HETATM		C3A		600		-26.605	14.439	1.00	0.00	HEM
		C4A		600		-26.338	15.849	1.00	0.00	HEM
HETATM				600		-25.288	17.964	1.00	0.00	HEM
HETATM		CIB					18.724	1.00	0.00	HEM
HETATM		C2B		600		-24.465		1.00	0.00	HEM
HETATM		C3B		600		-24.471	20.029			HEM
HETATM		C4B		600		-25.267	20.000	1.00	0.00	HEM
HETATM		C1C		600		-26.220	21.122	1.00	0.00	
HETATM		C2C		600		-26.398	22.303	1.00	0.00	HEM
HETATM		C3C		600		-27.105	21.896	1.00	0.00	HEM
HETATM		C4C		600		-27.359	20.473	1.00	0.00	HEM
HETATM		ClD		600		-28.419	18.358	1.00	0.00	HEM
HETATM		C2D		600		-29.229	17.581	1.00	0.00	HEM
HETATM	3727	C3D	HEM	600		-29.362	16.350	1.00	0.00	HEM
HETATM	3728	C4D	HEM	600		-28.591	16.366	1.00	0.00	HEM
HETATM	3729	CHA	HEM	600		-28.392	15.257	1.00	0.00	HEM
HETATM	3730	CHB	HEM	600	17.121	-25.582	16.615	1.00	0.00	HEM
HETATM	3731	CHC	HEM	600	18.841	-25.488	21.097	1.00	0.00	HEM
HETATM	3732	CHD	HEM	600	22.615	-28.078	19.676	1.00	0.00	HEM
HETATM	3733	CMA	HEM	600	16.761	-26.027	13.539	1.00	0.00	HEM
HETATM	3734	CAA	HEM	600	18.874	-28.152	12.738	1.00	0.00	HEM
HETATM	3735	CBA	HEM	600	19.655	-27.341	11.731	1.00	0.00	HEM
HETATM	3736	CGA	HEM	600	19.868	-28.082	10.424	1.00	0.00	HEM
HETATM	3737	Ola	HEM	600	18.997	-28.897	10.031	1.00	0.00	HEM
HETATM	3738	02A	HEM	600	20.918	-27.812	9.777	1.00	0.00	HEM
HETATM	3739	СМВ	HEM	600	15.130	-23.749	18.107	1.00	0.00	HEM
HETATM	3740	CAB	HEM	600	16.311	-23.874	21.208	1.00	0.00	HEM
HETATM	3741	CBB	HEM	600	15.206	-23.138	21.387	1.00	0.00	HEM
HETATM		CMC		600	20.479	-25.906	23.689	1.00	0.00	HEM
HETATM		CAC		600		-27.556	22.589	1.00	0.00	HEM
HETATM		CBC		600		-27.610	23.914	1.00	0.00	HEM
HETATM	-	CMD		600		-29.779	18.033	1.00	0.00	HEM
HETATM		CAD		600		-30.183	15.203	1.00	0.00	HEM
HETATM		CBD		600		-31.591	15.127	1.00	0.00	HEM
HETATM		CGD		600		-32.470	14.027	1.00	0.00	HEM
HETATM		01D		600		-33.625	14.347	1.00	0.00	HEM
HETATM		02D		600		-32.020	12.856	1.00	0.00	HEM
HIMIU	3130	J2 D	. Ed.	000	23.330	32.020				

#### Sequences:

SEQ ID N°1: P450 Nor, crystal structure 1rom

SEO ID N°2: P450 Ery F, crystal structure I oxa

SEQ ID N°3: P450 Terp, crystal structure 1cpt

5 SEQ ID N°4: P450 Cam, crystal structure 3cpp

SEQ ID N°5: P450 BM3, crystal structure 2hpd

The sequence corresponding to the PDB structure includes 471 residues. For more clarity in Figure 1, the last 12 residues have been omitted, the C-terminal part having no equivalent counterpart in the other structures aligned.

10 SEQ ID N°6: P450 2C5, crystal structure 1dt6

Cyp2C5 from Oryctolagus cuniculus (Rabbit), with membrane spanning residues 3-21 deleted and a 4 residue histidine tag at the C-Terminus containing additional internal mutations.

SEO ID N°7: P450 2C5 rabbit

Sequence corresponding to the non-mutated CYP 2C5 gene from Oryctolagus cuniculus (Rabbit), consistently with SwissProt CPC5\_RABIT P00179.

SEQ ID N° 8: CYP51, crystal structure 1e9x

Cyp51 from Mycobacterium tuberculosis, with a 4 residue histidine tag at the C-Terminus.

20 SEQ ID N°9: CYP3A1 rat

SEQ ID N°10: CYP3A3 human

Cytochrome P-450, a possible variant of CYP3A4, inducible by glucocorticoids in human liver.

SEQ ID N°11: CYP3A4 human

Numbering starts at Ala 1 (first residue Met is not included, consistently with SwissProt CP34\_HUMAN P08684)

SEQ ID N°12: CYP3A5 human

SEQ ID N°13: CYP3A43 human

SEQ ID N°14: CYP3A6 rabbit

30 SEQ ID N°15: CYP3A7 human

SEQ ID N°16: CYP3A12 dog

SEQ ID N°17: CYP3A29 pig

SEQ ID N°18: CYP3A13 mouse

- Figure 1: Structure-based alignment of human cytochromes P450 3A3, 3A4, 3A5, 3A7 and 3A43 and of selected mammalian P450 3A isozymes, with bacterial P450 crystal template structures and rabbit P450 2C5 crystal template structure.
- Sequence numbering is indicated for each enzyme of the structural template and for the human 3A4 and 3A7 isozymes, as examples given in the present invention. This alignment is first based on the structural alignment of bacterial P450s and rabbit P450 2C5 derived from GOK analysis. Human P450 3A sequences were then aligned with in-house tools that locates the CSBs on the target sequence. The alignment shown outside the CSBs is not relevant, as there is no structural information available in these regions. The CSB sequences are indicated by bold uppercase characters and are highlighted in grey. Amino acids strictly conserved between CYP3A and 2C5, or between CYP3A and all the sequences of crystal structures, are highlighted in black.
- Figure 2: Ramachandran plot of a lowest energy model of CYP3A4 produced by DYANA-XPLOR calculations from the six-template structural alignement. Figure 3: view of one optimized CYP3A4 model. This figure can be replaced by the whole set of coordinates file of table 3 in the PDB format.
  - Figure 4: final position of testosterone into the CYP3A4 and CYP3A7 active sites after soft-restrained dynamics docking. The active sites are characterized by six Substrates Recognition Sites (SRS, after Gotoh 1989, in bold) associated to fragments of secondary element structures (in italic).
  - Panel 4A In CYP3A4 active site, the docked testosterone molecule is oriented so that the A steroid cycle (carrying in position 3 a carbonyl function with an oxygen atom symbolized by a large ball ) is close to the heminic iron. This supports the propensity of CYP3A4 to metabolize testosterone in 6  $\beta$  position as indicated by the black solid arrow.
  - Panel 4B In CYP3A7 active site, the docked testosterone molecule is oriented so that the D steroid cycle (carrying in position 17 a hydroxylic function with an oxygen atom symbolized by a large ball ) is close to the heminic iron. This supports the propensity of CYP3A7 to metabolize testosterone in 16  $\alpha$  position as indicated by the black solid arrow

Figure 5: Energy profile of the soft-restrained dynamics docking of testosterone into CYP3A4 model.

#### Example 1: Determination of the 3D-structure of P450 3A4.

#### 5 Material

The coordinates of the six P450 crystal structures: P450cam (3cpp), P450terp (1cpt), P450BM-3 (2hpd), P450eryF (1oxa), P450 nor (1rom) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank. The structural alignment and the conserved regions determination were realized using the GOK software (Jean et al. 1997) running on an Octane Silicon-Graphics workstation. Structures were built using the DYANA (Güntert et al. 1997), and X-PLOR softwares (Brünger 1992). Docking studies were performed with SYBYL 6.6 (Tripos Inc.) and TRIPOS force field. The structures were analyzed using Procheck-NMR (Laskowski et al. 1993) and visualized under SYBYL 6.6 (Tripos Inc.).

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#### Common Structural Blocks (CSB) determination.

The first key point of this homology modeling study is the identification of the structural elements (hereafter designed as CSBs for Common Structural Blocks) conserved among the family of cytochromes P450 of known 3D structures, and the localization of these elements in the target sequence. These two tasks are performed using the GOK software (Jean et al. 1997), and are well described in a forthcoming article (Minoletti et al., Proteins, Structure, Function and Genetics, 2002). In brief, the basic idea of CSB identification by GOK is to use an internal coordinate representation –  $(\alpha, \tau)$  in our case (another representation of  $\phi$ ,  $\psi$  and  $\omega$  angles) – and to search for fragments in the six-template proteins having similar local trajectories in the internal coordinate space. GOK provides two adjustable parameters (the  $\alpha$ -mesh and the  $\alpha$ -margin) that define the tolerance on the comparison of the trajectories. These parameters were adjusted recursively to values ranging from 15 to 30° (α-mesh) and 1 to 3 (α-margin in mesh units). The evaluation of the quality of the match was measured using two multiple-way rmsd calculated in the cartesian coordinates space: mp-rms (the mean of all pairwise rms deviations) and s-rms (the mean of the deviations calculated with respect to a mean structure obtained from the average internal coordinates). For the different CSBs,

mp-rms value ranged between 0.3 and 4.9 Å in average, and s-rms between 0.04 and 2.4 Å.

# CYP3A4 sequence alignment and evaluation of the profile

The multiple sequence alignment derived from the CSB identification was then used to build a similarity profile. The profile is defined as a position-specific scoring table created from aligned gap-free segments such as CSBs (Jean et al. 1997). The alignment then consists in a search of the best match (as per the best score) between a CSB of sequences defined structurally (i.e. independently of the nature of the aligned residues) and several other sequences that are well-aligned and exhibit a high sequence identity. In the P450 3A subfamily, many proteins exhibit high sequence identity. We extended our profile search program to take this information into account, i.e. to align the profile with a pre-defined multiple alignment of the cytochromes P450 3A subfamily members sequences (Gotoh 1992; Nelson et al. 1996). The similarity score was calculated using BLOSUM62 matrix (Henikoff and Henikoff 1992). The in-house tool SmartConsAlign (Atelier de Bioinformatique, Université Paris VI) described in Jean et al. 1997, allows to move the consensus matrix along the multiple sequence alignment of P450 3A family, and computes for each position a score of similarity. The best alignment found of CYP3A4 on CSBs is shown in Figure 1.

Once the alignment is completed, the 3D model rebuilding process can incorporate the atom Cartesian coordinates of the template structures only for amino acids located in structurally conserved regions (*i.e.* the CSBs). The coordinates of any of the template structures can be used for determining the final template. In each CSB, amino acid positions have been renumbered according to the sequence of human P450 3A4. At a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the modeled (target) residue. When residues differ, only the coordinates of the backbone atoms are assigned (Cα), and sometimes Cβ when they exist. Side chains are rebuilt from libraries giving the most probable rotamers for each amino acid (see below). In some cases, it was possible to superimpose the positions of carbon atoms of lateral chains up to ranks γ and δ along the sidechain, thus explicitly defining a unique rotamer.

For amino acids located outside the CSBs (structurally variable zones that include generally loops), the rebuilding is more complex, and can be done only after rebuilding of structurally conserved zones. In the multiple structural alignment (Figure 1), the regions separating the CSBs bring no structural information at all. Short loops are rebuilt entirely, since solutions of acceptable geometry for atoms are in limited number, *i.e.* the lowest energy drives the selection of the good geometry. For longer segments, various structures are provided by the constrained minimization runs, and a manual selection is operated.

#### 10 Constraints derivation and rebuilding

A strategy inspired of the techniques commonly used to built structures from NMR data (Patard et al. 1996) is applied. The main idea is to express all available information issued from the comparison of the templates in term of geometrical constraints (distances and angles). Each constraint will be defined as an interval (for a given pair of atoms, this is the average of the six atom-atom distances found in the template structures +/- the standard deviation), similarly to the strategy developed by Havel and Snow (Havel and Snow 1991). However, the number of constraints corresponding to all atom-atom distances, for example, would be prohibitive for a protein of the size of the P450 (around 1,000,000 inter-residual distances if we consider 250 conserved residues and an average of four atoms per residues). Previous NMR studies (Patard et al. 1996) have shown that local constraints are sufficient to allow a correct reconstruction of a structure. This reduces drastically the number of constraints needed, and increases the flexibility of the model. In addition, similarly to what is done in protein structure determination by NMR, we can build a family of structures instead of a single model. This allows an easier analysis of the well or less well-predicted regions. This is also an advantage for the analysis of the side-chain positions, particularly in prevision of a substrate docking study. Finally, the loops are passively reconstructed with the rest of the structure. The only specific information we have introduced in variable regions was to guide all their residues to an allowed region of the Ramachandran diagram. Indeed, analysis of well-defined structures shows that nearly all residues, including those of the loops, should belong to an allowed region. The lower the proportion of residues

found outside the allowed Ramachandran regions, the better the structure is. This criterion of quality has been applied to derive the model described herein.

Accordingly, we retained for model rebuilding all the distance and angle intervals corresponding to the following principles:

- all distances for which the lower boundary was less than 8 Å. This cutoff is totally sufficient to ensure, at least, the formation of the local structure elements. Such a cutoff is relatively high and thus costly in terms of size of constraints file, but proved necessary to ensure good results for the P450s. This may be due to the fact that P450 enzymes are mostly formed of α-helices, the average distance between two helices being larger than between two adjacent β-strands. In addition, the percentage of residues located outside CSBs is rather high in the structural alignment of P450s, and a better convergence can be obtained only at the expense of a high number of rebuilding distance constraints.
  - all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
  - finally, all the distances involving atoms of the heme group, to fix as much as possible the neighborhood of the iron atom.

The total number of distance constraints was, in these conditions, equal to 58506. Similarly, angular constraints were calculated in each building block. A CSB is indeed defined as a conserved trajectory in the  $\varphi, \psi$  coordinates space (or  $\alpha, \tau$ ). Thus, dihedral angles  $\varphi$  and  $\psi$  of all residues located in CSBs can be defined as constraints, given by the average values of corresponding  $\varphi, \psi$  angles in the six templates +/- the standard deviation. To these backbone dihedral angles, can be added the side chains torsion angles  $\chi_1, \chi_2$  whenever possible, as determined by the rotamer selection. The total number of dihedral angle constraints was, in these conditions, equal to 761.

#### Rotamer selection

In proteins, the preferential orientation of the side chain  $(60^{\circ}, -60^{\circ}, 180^{\circ})$  depends on the local conformation of the residue, and thus on the nature of the secondary structure in which the residue is involved. According to the rotamer library built by Karplus and coll. (Dunbrack and Karplus 1993), to a given  $(\varphi, \psi)$  couple in the

Ramachandran diagram can be associated a specific rotamer for each type of residue. These tables have been used to determine the most probable rotamer for each residue located in CSB, except when there are conserved atoms in the side chain that assign unambiguously a rotamer  $(\chi_1, \chi_2)$ . The selected  $(\chi_1, \chi_2)$  couples were included in the above-mentioned set of angle 761 dihedral constraints.

## Structure calculation and optimization

We used a procedure similar to structure calculation starting from NMR constraints. A first set of structures was calculated using the DYANA software (Güntert et al. 1997) and the 58506 distance and 761 angular constraints. Families of structures are generated. The energy of each structure is minimized with the procedure vtfmin in DYANA.

Due to the size and the amount of loops in the molecule, some structures presented topological defects and were discarded. The others were further optimized by using the X-PLOR software. A set of constraints was added at this stage in order to guide the loop residues to the nearest allowed region in the Ramachandran diagram. The topology and parameter files of CHARMM22 were used. The electrostatic term was turned off.

The DYANA software is unable to deal with disconnected objects. A new residue type was, thus, added to the standard amino acid library to take into account the the presence of the heme. This residue was obtained by combining the heme to a cysteine and was inserted at position 441 in the sequence of the protein (Figure 1).

### **Description of the CYP3A4 Model**

We rebuilt a model of the protein depleted of its first 50 residues (N-terminal domain). This segment is highly hydrophobic, and supposed to form the anchor of the protein in the membrane. There is no structural information about this putative transmembrane domain, and this segment was thus not incorporated into the modeling process, and in the final model. Such a "free" segment (with no constraints) would perturbate the convergence of computation or the stability of the whole rebuilt structure.

The quality of the various structures optimized under XPLOR was checked for the stereochemical quality (backbone and side chain conformation) by PROCHECK

(Laskowski et al. 1993). The Ramachadran plot shows that our six-template approach generated converging models, possessing the same fold. The lowest energy models had 73% of their non-glycine and non-proline residues with  $\varphi$ ,  $\psi$  conformation in the most favoured regions of the Ramachandran plot (core region), 20% in additional allowed regions, and 5% in the generously allowed regions. Only 2.3% (9 residues) had their  $\varphi$ ,  $\psi$  conformation in disallowed regions (Figure 2). The total number of residues in the model is 452; which 399 are non-glycine and non-proline residues, and number of residues in the native sequence is 502.

When compared to the CYP2C5 crystal structure, it can be noticed that the CYP3A4 model exhibits a good 3D similarity in the global fold than expected, since this structure counts only for one in the six-template approach. This proves that in this approach, there is no "averaging" effect, *i.e.* the mammalian structure had a decisive influence over the five bacterial (and fungus) templates. Our final fold of CYP3A4 is very consistent with a mammalian one, despite the fact that it has been rebuilt by using the structural information contained in non-mammalian cytochromes P450.

The active site is delimited by the six substrate recognition sites (SRS) that have been first identified and described by Gotoh (Gotoh 1992) from the unique structure available in the early 1990s (P450cam), and that are today commonly accepted for depicting substrate recognition by various cytochromes P450 (especially from the family 2, but extended to other P450 families). These sites are associated with the active site and are located in the less conserved regions of the CYPs, thus possibly accounting for the various substrate specificity among P450s. When comparing our various optimized structures, it is found that SRS1 (100-125, includes helix B), SRS 2 (205-218, includes C-terminus of helix F), and SRS3 (237-249, includes Nterminus part of helix G) are located in less-defined regions, with significant variability in spatial position (flexibility). These regions correspond also to parts of the sequence that are less well-aligned. At the opposite, the SRS4 (295-320, central part of helix I), SRS5 (363-380, C-term of helix K and β-sheet β1-4) and SRS6 (470-490,  $\beta$ -sheets  $\beta$ 4-1 and  $\beta$ 4-2) are well-defined fragments of the structures. SRS4 and SRS5 segments in particular are correlated to regions in the sequence that are unequivocally aligned.

The only model structure of CYP3A4 that has been described in the literature and that we can handle for structural comparison, is that of Szklarz and Halpert, derived from a multiple-template approach (four-bacterial template) (Szklarz and Halpert 1997). Roughly, the same secondary structures are identified, but we found divergences in SRS location between their model and those derived from the present approach. SRS4 and SRS5 match well, but SRS2 is shifted (divergence in the position of helix F along the sequence), while SRS1 (helix B'), SRS3 (helix G) and SRS6 (sheet β4) are more notably displaced. The loops connecting the secondary structures of these SRS significantly disagree. These differences are likely to issue from a wrong alignment with the crystal P450 structures in the model of Szklarz and Halpert.

# Example 2: Determination of the 3D-structure of P450 3A7.

The model rebuilding of CYP3A7 was performed according to the techniques described above in example 1 for CYP3A4, except that we used a restrained set of four-template structures, still including the mammalian CYP2C5, in order to test the robustness of the modeling approach. Below are pointed out only the differences in input data and the results relevant to CYP3A7.

#### 20 Material

The coordinates of the four P450 crystal structures: P450BM-3 (2hpd), P450eryF (1oxa), P450 51-like from *Mycobacterium tuberculosis* (1e9x) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank and used as initial template for GOK analysis.

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# Common Structural Blocks (CSB) determination.

The GOK parameters were adjusted recursively to values ranging from 10 to 30° (α-mesh) and 1 to 3 (α-margin in mesh units). Occasionally, the α-mesh value was pushed up to 60° to refine some local structured loops (DE loop, HI loop) or short helices (such as J'). 27 CSBs have been identified. New CSBs were detected: the block 7\* (between blocks 6 and 7A), the block 7B\* (between 7B and 8) and the block 7C (between 7B\* and 8). For the different CSBs, mp-rms value ranged between 0.12 and 4.57 Å in average.

The best alignment found of CYP3A7 on CSBs is shown in Figure 1. On the 459 residues comprised in the model structure (the protein was rebuilt depleted of its first 44 residues from the N-terminal domain), 337 residues were found located in CSBs, i.e. 73% of residues belong to structurally conserved regions of the four-template set.

## Constraints derivation and rebuilding

With a larger cutoff (12 Å), we obtained around 73000 distance constraints, and 900 dihedral constraints.

The residue covalently linked to the heme group is at position 442 in the sequence of the protein (Figure 1).

# Description of the CYP3A7 model

The four-template approach generated converging models, possessing the same fold. The PROCHECK analysis for structure quality assessment for the lowest energy models showed 74.4% of their non-glycine and non-proline residues with  $\varphi$ ,  $\psi$  conformation in the most favoured regions of the Ramachandran plot (core region), 18.2% in additional allowed regions, and 4.7% in the generously allowed regions. 2.7% (11 residues) had their  $\varphi$ ,  $\psi$  conformation in disallowed regions. The total number of residues in the model is 459; which 407 are non-glycine and non-proline residues, and number of residues in the native sequence is 503.

A closer inspection of the structure, and after the results of dynamics docking experiments (see below), revealed that several hydrogen bonds can hinder the main access to the active site. Thus, key residues that are likely to be involved in the recognition and admission of the substrate are Q79; F102; R105; R106; F108; F248; F304 and E374, and additionally C98 and C377 (Figure 4B). More specifically, R105, R106, Q79 and E374 can establish mutual hydrogen bonds in one of the access channels, and are thus involved in the access of the substrate towards the active site.

## **Example 3: Docking Strategy**

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Our aim in this example was to obtain the different positions of the known substrates of CYP3A in the active site, consistent with the oxidation sites and

biochemical differences among the CYP3A isoforms. Considering the fact that the heme-binding site is deeply buried in the protein structure, and thus the selection and the pathway of the substrates within the enzyme structure are strongly dependent on the various possibilities of structure opening, we implemented a special approach more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained dynamics docking". This technique employs constrained molecular dynamics simulations, where the only constraints are heme-substrate distances. The successive steps are:

### 10 Conversion of the PDB XPLOR file in PDB for SYBYL file

The optimized structures with XPLOR (PDB format) are visualized with the SYBYL 6.6 software (Tripos Inc.), which implies a conversion of the file (atoms types correction) so as to make it compatible and exploitable in the constrained dynamics which will be performed with SYBYL.

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# Stabilization of the P450 3A4 model generated under XPLOR

Then, we do agregate N°1 (in the meaning of SYBYL) with all the  $NC_{\alpha}CO$  atoms of the peptide backbone of the protein. The structure is relaxed with a dynamic of 10ns at 100K followed by a minimization of 100 steps. Agregate N°1 is then deleted.

We do agregate N°2 constituted of the protein  $C_{\alpha}$  only. The protein relaxation is reiterated with a dynamic of 10 ns at 100K and a minimization of 100 steps. Agregate N°2 is then deleted.

The all protein is then relaxed with a first dynamic of 1ns at 100K, followed by a dynamic of 1ns at 200K and a dynamic of 10ns at 300K. We terminate with a minimization of 100 steps.

# Restrained dynamics docking of the substrate (example: testosterone)

We do agregate N°3 constituted of all atoms outside a sphere of 20Å around the  $C_{\alpha}$  of residues constituting the heart of the B' loop. We also add heminic iron to this aggregate.

The substrate is placed inside the protein, at around 30Å from the heminic iron and next to SRS1 and SRS5 sites. The substrate is placed so that the contraints between

the heminic iron and the substrate backbone go between SRS1, SRS5 and SRS3. Thus, for testosterone docking, we establish 4 distance contraints (limit below 3Å, above 10Å) between heminic iron and C3, C8, C10 and C13 carbons with a constraint of 2 kcal/Å on the entire structure so as to avoid to favour the approach of one part of the substrate more than the other.

We begin to perform a dynamic without contraints of the entire system at 20 K during 2ns to stabilize the system, then we perform a dynamic under contraints at 20 K during 5ns. We observe that the substrate worms between SRS1, SRS3 et SRS5 to reach a position at the vicinity of heminic iron. We terminate with a dynamic without contraints at 300 K to relax the system and we realize a minimization of 1000 steps.

#### Results

We found that the testosterone molecule is positioned at the vicinity of heminic iron in such way that the C6 of testosterone be at 4.9Å of the iron, which is compatible with the hydroxylation of this compound to give  $6\beta$ -hydroxy-testosterone (Figure 4A).

Minimizations and dynamics with the SYBYL software are performed with the Tripos force field following the parameters: dielectric constant equal to 1 and distance-dependent, minimization method of POWELL, a minimum gradient of 0.05kcal.mol<sup>-1</sup>.Å<sup>-1</sup>, electrostatics charges calculated according to the Gasteiger-Hückel method, and a NB cutoff of 8.0Å (non-bond energies). The energetic diagram of dynamic docking of testosterone is shown in Figure 5.

#### 25 Interest of this docking strategy:

Most P450 isozymes recognize only one substrate (for specific catalysis in a metabolic pathway), or a very limited number of substrates, all chemically closely related. At the contrary, CYP 3A isozymes are known to recognize a large palette of substrates, and are also capable of multiple binding in the active site, up to three molecules in the vicinity of the heme, according to the model developed by Hosea et al. 2000. Multiple pharmacophoric behavior (Ekins et al. 2003), as well as allosteric or synergistic effects, characterize the members of this P450 subfamily.

The docking strategy described above can be easily extended to different binding and metabolism scenario.

For example, the docking of two or three testosterone molecules, or of two testosterone molecules and one alpha-naphtoflavone molecule ( $\alpha NF$ ) can be simulated in the following manner:

- In a first step, a testosterone molecule is dynamically docked under constraints, and then released of its constraints to freely evolve in the active site and find a first bound equilibrium position.
- In a next step, an external testosterone is presented, at the same entrance of the protein structure or in the vicinity of another access channel, and then dynamically docked under constraints. The system first evolves under constraints applied to the second molecule, and can be released for a subsequent free MD simulation of the two molecules bound in the active site. One can see the first bound molecule (testosterone or another substrate) to be re-oriented under the effect of the second docking, simulating a situation of cooperativity.
- Similarly, the second molecule docked can be different from the first bound, e.g.. a first testosterone bound to the active site followed by the docking of an  $\alpha NF$  molecule, or the reverse situation.
- One can combine of course the possibilities: for example, two molecules (identical or of different chemical nature) are docked following the two steps above, and then, after stabilization around an equilibrium position, a third molecule is introduced under constraints, and then released from its constraints to let the system evolving towards a favorable energetic conformational state. In this way, two  $\alpha NF$  and one testosterone or one  $\alpha NF$  and two testosterone can be docked.
- Of course, not only substrates can be docked, but also inhibitors. The docking procedure above can help to measure the potential inhibitory power of a molecule, for example a compound comprising an imidazole group. A first step would include a standard constrained dynamic docking of the potential inhibitor, followed by a free MD simulation (constraints are released when the inhibitor is in the active site), or by a specifically-constrained MD simulation where the imidazole group is confined in the vicinity of the heminic iron by using an additional distance constraint Fe-imidazole. In a following step, a second substrate is dynamically docked under constraints from the exterior, and one can determine in what

conditions the second molecule can chase the first one from its binding position. The strength of the additional constraint can be a measurement of the inhibitory potential.

Correspondingly, the exit pathway of the metabolites can be explored by simulating the exit of the molecule bound to the active site, using either free MD simulation (if the chemical nature of the transformed molecule allows an energetical instability), or using inverted constraints, *i.e.* soft distance constraints (between an external point and the bound molecule) that help to expel out the metabolite. Additionally, the best exit pathway can be deduced from the most favored energy profiles.

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### **Claims**

- 5 1. A method for designing a 3-dimentional (3-D) model of a protein, the 3-D representation of at least three family members has already been experimentally obtained, [said 3-D representation presenting similarities], comprising the steps of:
  - a. identification of common structural blocks (CSBs) among said members of said family,
- 10 **b.** alignment of the amino-acids primary sequence of said family members according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
  - c. alignment of said protein as compared on said first alignment, in order to obtain a second alignment, wherein:
- i. alignment of said protein is performed in order to optimize the amino-acids alignment between said protein and said first alignment, when one or more consensus amino-acid exists in said aligned CSBs in said first alignment, and in the amino-acid sequence of said protein, said consensus amino-acids are anchors of said second alignment,
- 20 ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible in out-of-block regions, if better to align the primary amino-acids sequences,
  - d. definition of the 3-D structure of CSBs of said protein, according to the 3-D structure of the CSBs of said family members,
- e. definition of the global constraints (distance and angular constraints) derived from the comparisons of the structural templates in CSBs, and definition of the local constraints (distance and angular constraints) for the atoms of residues that are not structurally determined after step d. (that are not in the CSBs),
  - f. selection of rotamers,
- 30 g. determination of a family of 3-D model structures of said protein, taking into account said 3-D structure of CSBs obtained in step d., said global and local constraints defined in step e., and said rotamers defined in step f.,
  - h. optimization of said family of 3-D models obtained in step g., by

- i discarding structures that present topological defects, and
- ii recalculating 3-D structures by taking electrostatic forces into account,
- and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment,
- 5 when the obtained model structures do not satisfactorily account for known mutations having biological effects.
  - 2. The method of claim 1, wherein said 3-D representation of family members has been obtained by crystallography or NMR.
- 3. The method of claim 1, wherein said alignment of said CSBs in step b. is performed by use of the GOK software.
  - 4. The method of claim 1, wherein said alignment of said CSBs in step c. is performed by use of the GOK software.
  - 5. The method of claim 1, wherein step d. is performed according to the following rules:
- 15 i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the target residue,
  - ii. When residues differ, only the coordinates of the backbone atoms are assigned  $(C\alpha)$ , and sometimes  $C\beta$  or  $C\gamma$  when they exist.
- 20 6. The method of claim 1, wherein said definition of local constraints in step e. is performed by analysis of the allowed regions in Ramachandran diagram.
  - 7. The method of claim 1, wherein global and local constraints are selected in step e. by the following rules:
  - i. all distances for which the lower boundary was less than 8 Å.
- 25 ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
  - iii.all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom.
- 30 8. The method of claim 1, wherein angular constraints are selected in step e. by the following rule:

- i. dihedral angles  $\phi$  and  $\psi$  of all residues located in CSBs are defined as constraints, given by the average values of corresponding  $\phi$ ,  $\psi$  angles in said family members +/- the calculated standard deviation.
- 9. The method of claim 1, wherein said rotamers in step f are selected from the couples according to the tables of Dunbrack and Karplus, where the choice of rotamers of a given amino acid is guided by the most favored zones in Ramachandran  $\chi_1$ ,  $\chi_2$  maps.
- 10. The method of claim 1, wherein said step g. is performed with the DYANA software.
- 10 11. The method of claim 1, wherein said optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brunger, X-PLOR, version 3.1.
  - 12. The method of claim 1, wherein said protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A.
- 13. The method of claim 12, wherein said mammal cytochrome P450 3A is
  5 selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
  - 14. The method of claim 12, wherein said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).
- 15. The method of claims 1 and 14, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A4 are chosen from Nor (SEQ ID N° 1), Ery F (SEQ ID N° 2), terp (SEQ ID N° 3), Cam (SEQ ID N° 4), BM3 (SEQ ID N° 5) and 2C5 (SEQ ID N° 6).
  - 16. The method of claims 1 and 14, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A7 are chosen from Ery F (SEQ ID N° 2), BM3 (SEQ ID N° 5), CYP51 (SEQ ID N° 8) and 2C5 (SEQ ID N° 6).
    - 17. A 3-D structure model of a protein, obtained by the method according to claim 1.
- 30 18. The model of claim 17, wherein said protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A.

- 19. The model of claim 18, wherein said mammal cytochrome P450 3A is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
- 20. The model of claim 18, wherein said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).
  - 21. The model of claim 20, wherein said protein is a cytochrome P450 3A4 or 3A7.
- The model of claim 21, wherein the residues C97; R104; F101; F107; F247;
  F303 and C376 are involved in the CYP 3A4 for the recognition and uptake of the substrate at the entry site, and its binding into the active site.
  - 23. The model of claim 20, wherein the residues Q79; F102; R105; R106; F108; F248; F304 and E374 are involved in the CYP 3A7 for the recognition and uptake of the substrate at the entry site, and its binding into the active site.
- 15 24. The model of claim 22, having the 3-D atomic coordinates of Table 3.
  - The model of claim 23, having the 3-D atomic coordinates of Table 4.
  - 26. A method for designing a protein, biological functions of which are altered, comprising:
  - a) obtaining a 3-D model of said protein by the method of claim 1,
- 20 b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
  - c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.
- 25 27. A computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps of
  - j. determining a force field, and independently simulating the presence of said enzyme in said force field,
- structure, wherein the spatial position of some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by i. simulating an increase in temperature (in order to give kinetic energy),

- ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- 1. optionally repeating step k in order to obtain other Ep minima, wherein said Ep minima are such that the structure of the protein remains folded,
- 5 m. minimizing Ep in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by
  - i. simulating an increase in temperature (in order to give kinetic energy), and
  - ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
  - n. simulating, at 0 K the presence of said substrate next to said enzyme,
- o. optionally generating a molecular dynamics simulation on said substrate and enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)
  - p. generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- q. generating a molecular dynamics simulation on said substrate and enzyme, with said constraints imposed in step p.,
  - r. optionally, generating a molecular dynamics simulation on said substrate and enzyme without said constraints of step p.
- 28. The method of claim 27, wherein said fixed atoms in step **k**. are the backbone atoms N-Cα-CO in the first minimization step and only Cα in subsequent minimization steps.
  - 29. The method of claim 27, wherein said kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
  - 30. The method of claim 27, wherein said force field in step j. comprises forces linked to
    - a. the distance between atoms,
    - b. the angles of valence,
    - c. the dihedral angles,
    - d. the deformation with regard to planar geometry,
- 30 e. the electrostatic field,
  - f. the Van der Waals forces,
  - g. hydrogen bonds.

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- 31. The method of claim 27, wherein said constraints in step **p.** are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site.
- 32. The method of claim 31, wherein said constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
  - 33. The method of claim 27, wherein step o. is performed with a simulated temperature of between about 15 and 50 K.
- 34. The method of claim 27, wherein step q. is performed with a simulated temperature of between about 15 and 50 K.
  - 35. The method of claim 27, wherein step r. is performed with a simulated temperature of between about 200 and 350 K.
  - 36. The method of claim 27, wherein said enzyme is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes.
- 15 37. The method of claim 36, wherein said cytochrome is a cytochrome P450 3A4, and said structure is the structure obtained by the method of claim 15, in particular the model structure of claim 22.
  - 38. The method of claim 36, wherein said substrate is a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).
  - 39. The method of claim 38, wherein said substrate is testosterone.
  - 40. A computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a 3-D structure of which is available, comprising the steps consisting of performing the steps depicted in claim 27 with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained state after molecular dynamics simulation..
  - 41. The method of claim 40, wherein the first and second substrates are the same molecule.
  - 42. The method of claim 40, wherein the first and second substrates are different molecules.
    - 43. The method of claim 41, wherein the first and second substrates display an allosteric effect.

- 44. The method of claim 41, wherein the first and second substrates display a synergistic effect.
- 45. The method of claims 41 and 42, wherein at least one of the substrates is an inhibitor or display an inhibitor-based mechanism.
- The method of claims 41 and 42, wherein at least one of the substrates is an agonist.
  - 47. The method of claim 40 comprising successively repeating the steps of claim 20 with a 3<sup>rd</sup>, 4<sup>th</sup> or 5<sup>th</sup> substrate, some of them being the same or different molecules.
- 10 48. The method of claim 40, wherein said fixed atoms in step k. are the backbone atoms N-Cα-CO in the first minimization step and only Cα in subsequent minimization steps.
  - 49. The method of claim 40, wherein said kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.
- 15 50. The method of claim 40, wherein said force field in step **j**. comprises forces linked to:
  - a. the distance between atoms,
  - b. the angles of valence
  - c. the dihedral angles,
- 20 d. the deformation with regard to planar geometry,
  - e. the electrostatic field,
  - f. the Van der Waals forces
  - g. hydrogen bonds
- 51. The method of claim 40, wherein said constraints in step **p.** are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site.
  - 52. The method of claim 51, wherein said constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- 30 53. The method of claim 40, wherein step o. is performed with a simulated temperature of between about 15 and 50 K.
  - 54. The method of claim 40, wherein step q. is performed with a simulated temperature of between about 15 and 50 K.

- 55. The method of claim 40, wherein step r. is performed with a simulated temperature of between about 200 and 350 K.
- The method of claim 40, wherein said enzyme is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A.
- 5 57. The method of claim 56, wherein said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the method of claim 15, in particular the model structure of claim 22.
  - 58. The method of claim 40, wherein said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A).
  - 59. The method of claim 58, wherein said substrate is testosterone.
  - 60. The use of the method according to claim 27 or 40 for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.
- 15 61. The use of the method according to claim 40 or 47 for determining the effect of a first substrate on a second substrate.
  - 62. The use according to claim 61 applied to pharmaceutical products.
  - 63. The use of the method according to claim 40 or 47 for determining the effect of a first testosterone molecule on a second testosterone molecule.
- 20 64. The use of the method according to claim 40 or 47 for determining the effect of a first testosterone molecule on a second alpha-naphtoflavone molecule.
  - 65. The use of the method according to claim 27 to 47 for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate.
- 25 66. The use of the method according to claim 27 to 39, or 40 to 47, for performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the computed simulation.
  - 67. The use of the method according to claims 27 to 39, or 40 to 47, to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to determine if the exit of the given metabolite from the enzyme is favored or not.

2 Ery F (lox. 3 Terp (lcp 4 Cam (3cp) 5 BM3 (2hp) 6 2C5 (ldt 7 CPC5 RABIT	dllsaltlet wvllavslvl alipdlamet wllavslvl mdlipnfamet wvlatslvl mdlipsfstet wllaislvl mdlipsfstet wllaislvl mdlipsfstet wvllatslvl mdlipnfsmet wvlatslvl mdlipsfstet wvllatslvl mdlipnfsmet wwllatslvl	mda snanlaplpptmakkt lllsiwkqnsms lygfgtrthg lylygthshg lylygthshg lylygtrthg lyiygthshk lylygtrthg lyiygthshk lylygtrthg lylygtrthg lylygtythg lylygtythg	ratipehiar tvilpqgyad hvpehlvfdf dmynpsnlsa ikempqpktf gelknlplln sskgklpoor tafgiignil grgkl-page tafgiignil avalprvsig hdehghleef lfkkqgi som talaffgtvillfkklgi som talaflgnil triklgi som talaflgnil lfkklgi som talaflgnil trikklgi som talaflgnil	( 16 ) ( 13 ) ( 23 ) ( 36 ) ( 21 ) ( 25 ) ( 43 ) ( 22 ) ( 50 )
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	dWIST TAET reta d-ev	PUTEURE PLAMAHTEGY DLYWTRCNG- ETERFEAL-G PYFTYTICMK PVFTYTICMK DVGTFOEA-G KIWGLEDGGM KVWGFYDGGG KVWGEYDGGG KWWGLYDGGG KWWGLYDGGG KWWGLYDGGG KWWGLYDGGG KWWGYYDGTG KWWGYYDGTG	SLAWLVIKER DVCFVatse- quawlvicto Earaalsdl- dewilatkie Dvmolgkqpg chwlatkie Dvmolgkqpg rvtrilsor likeac-des -Etvilegte Avkea vdlg -Etvilegte Avkea vdlg kovvilsgshanefff-rag -Elfaitdte Miknvlykec -Vlaitdpd Miktvlykec -Vlaitdpd Miktvlykec -Evlaitdpd Miktvlykec -Elmvitdpd Miktvlykec -Elmvitdpd Miktvlykec -Elmvitdpd Miktvlykec -Evlaitdpd Miktvlykec	(58) (54) (68) (79) (67) (73) (91) (66)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	rlssdpkkky pgvevefpay lfsnaegse hfssecpfi rfdknleefagr eefagt dddldq ysvftnysvftnysvftn ysvftnysvftnysvftnysvftn	IgfPEDVRN- IJYDQNNEAF IJYDQNNEAF	aka -kpTFVDVDRy fatNMGTSDR mrsisggcph vidSLTSMDR ydfIPTSMDR r	( 91 ) ( 94 ) ( 107 ) ( 105 ) ( 91 ) ( 98 ) ( 117 ) ( 92 ) ( 122 )

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1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	PEHMHORS MVEPTETPEA VKnLOPYLLORTVDDLLEG MKOKGCANGPPTHTRIRK LVSQEETVITVEAMR PRVEQITAEL LDEVGdS-GVPTHTAYRG LTINWEGPAS iI	( 150 ) ( 147 ) ( 138 ) ( 145 )
	CSB 2A CSB 2B	
1	VOLVKEFALP-VPSYMIYTLLEGVPFNDLEXLETCONAIRT	( 177 )
2	VDTVDRFAHP-EPEKVICELLE GVDEAARGAF GRWSSELLVM	( 176 )
3	COPMIDICALY YPI:HVVMTAL GVPEDDEPLM LKLTODFFGV	(190)
4	CNFTEDYAEP FPIREFMILA GLP EEDIPHL KYLTDOMIP	(187)
5	TEVPEDMTRL TILDTE GLCGT NYR fnsfyrd qph PFITSMV RALDEAMN kl CDPTFILGCA PCNV CSVIS HNR fdykd EEFLKIM ESLHENVEll	( 188 )
6	COPTFILGCA PCNYACSVIE HNRfdykdEEFLKIM ESLNENVRIL	(208)
7 8	TOULDFFARE TIXTSSACLE GKKFrd qldGRFAKLY HELERGTDpl	(179)
9	VIMKKVFGAY SMDWITSTS GVNvdslnNPKDPFV EKTKKLLRfd	
10	www.knurcay gmnumrsssi cunudslnNPODPLV ENTKKLLRfd	
11	VTLKDVFGAY SMDVETSTSHEGVNidsln NPODPFV ENTKKLLRfd	( 213 )
12	INTERPOLATION OF THE PROPERTY	
13	INLKDFFGAY TMOVETGTLE GVNldslnNPQDFFL KNMKKLLKld VDLKEIFGAY SMOVETGTSE GVNidslrNPQDPFV KNVRRLLKfs	
14	VILKHVECAY SMDVETSTSE GVNids1 NPODPFV ENTKKLIRE	(214)
15 16	INLKDVFGAY SMDVITSTSE GVNidslnHPQDPFV ENTKKLLKfd	( 211 /
17	VIMKDIFGAY SMDVATSTAE GVNidslnNPQDPFV ENSKKLLKfs	
18	TSMKDIFGAY SMDYATATSE GVNidsln NPQDPFV EKIKKLLKfd	
	CSB 3 CSB 4	
•		•
		( 204 )
1	dp eraeqRCOAATREVVNFILDL VERRET	(204)
2	eaarreneTi=ATEYDYFNGF TVDRRS	(216)
3	dg smtFAEAK EALYDYLIPI TEORRO	(213)
4 5	qranpdd -payd enkrqFOEDI KVMNDLVDKI IADRKAs	( 226 )
6	gtpwlqvynn fpalldyfp- gihktlikna Diknfimek vkehokl-ld	(238)
ž	sspwlgyvnn fpalldyfp- gihktLKNA DYIKNFIMEK VKEHEK1-ld	(256)
8	avvdpvl -pi esfrrpear NGIVALVADI MNGRIAnp	(216)
9	ffdplfls vvlfpfltpi yemlnICMFP KDSIEFFKKF VYRMKEtrld	
10	fldpffls itvfpflipi levlnICVFP REVTNFLRKA VKRMKEsrle	, aca s
11	fldpffls itvfpflipi levlnICVFP REVINFLRKS VKRMKEsrle	( 261 )
12 13	fld-plfls iilfpfltpv fealnVSLFP KDTINFLSKS VNRMKRsrln fld-pflll islfpfltpv fealnIGLFP KDVTHFLKNS IERMKEsrlk	
13	ffdpllls itlfpfltpi fealhISMFP KDVMDFLKTS VEKIKDdrlk	
15	pldpfvls ikvfpfltpi lealnITVFP RKVISFLTKS VKQIKEgrlk	(262)
16	fldpfffs illfpfltpv feilnIWLFP KKVTDFFRKS VERMKEsrlk	
17	ffdpflls liffpfltpi fevlnITLFP KSSVNFFTKS VKRMKEsrlt	
18	ifd-plfls vtlfpfltpv fdalnVSLFP RDVISFFTTS VERMKEnrmk	
	CSB 5	

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1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	epddil salisyqdddcpkdbym salisyqdddcpkdbym salisyqdddcpkdbym salisyqdddcpkdbym salisyqdyngeqsdbil thmingkdpennprofil DCFLlkmeqennprofil DCFLlkmeqe ptdksdromi DVIIA-vkae syqkhryofi QIMMNahnds dtqkhryofi QIMIDsq-ns dkqkhryofi QIMIDsq-ns dkqkhryofi QIMIDsq-ns dkqkryofi QIMINsq-ns etqkhryofi QIMINsq-ns dqkrryofi QIMINsq-ns nkekqryofi QIMINsq-ns nkekqryofi QIMINsq-ns nkekqryofi QIMINsq-ns	-dggngr t-ge nn1 t-gt keteshk keteshk keteshk keteshk ketkshk ketkshk ketkshk ketdhk kemdthk kemdthk	rLSADELTSIS yidDKYINAY piTSDEAKRMI plDDENIRYO efTLESLVIA rfSADELTVAQ alSDLELVAQ	ALVILLAGER  VALATAGHD  COLLLAGED  COLLLAGED	( ; ; ; ; ; ; ; ; ; ; ; ; ; ; ; ; ; ; ;	242 243 254 251 267 279 297 259 307	) ) ) ) )
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	TWONTALGY ATTACHED ASSUME TO THE TOTAL THE TOTAL THE TOTAL TO THE TOTAL TO THE TOTAL T	LATAKS ROELTE LOKAAR - aa AARVOE - er AARVOE - lot QKKLOE - ld QKKLOE - ld QKKLOE - ld QKLOE - ld	rvlvdp-vps vigrhrs-pc vigrhrs-pc elygdgrsvs alpnka-ppt vlpnka-ppt vlpnka-ppt vlpnka-pvt llpnka-pvt llpnka-ppt tfpnka-lpt tfpnka-ppt	dpani yedelegali ykqvkqlkyy ykqvkqlkyy mqdrsrmyyr fhalrqiyor ydtvmemeyr ydtvlqmeyr ydtvlqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr ydalvqmeyr		272 273 284 281 314 327 345 307 355	)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	PORVEELCRY HTASalaiku PRAVEETIRT IAPPet-tip PRAVEETIRT IAPPet-tip PRAVEETIRT IAPPet-tip PRAVEETIRT PSLVa-dGP GWYNEALRI WPTAP-afSI BAVTHEIORF IDLLptnlpp BAVIHEIORF IDLLptnlpp ENVIRETIRT HPPLI-ilm DMVNETIRT FPIAMT-lef DMVNETIRT FPVAMT-lef DMVNETIRT FPVAMT-lef DMVNETIRT FPVAMT-lef DMVNETIRT YPIAGT-lef	TALADTEVRO TITSDYEFHO TAKEDTYLOG TAVTROVEFRO VOKKOVEINO	-ONIKREDRI -VOLKKEDOI -VOLKKEDOI -VELKEDEI -VELKETDI -HRIHEGDLV -WEIDKGVVV -WEIDKGVVV -VELKESMV -VELKETIV -VELKETVV -VELKETVV	MISYPSANRO LIPOMISCIO MYLIPOMISCIO MYLIPOMINO ITSITSVIHO ITSITSVIHO ASPAISNRI MIPSYALHRO MIPSYALHRO MIPSYALHRO MYPTYALHRO MYPTYALHRO MYPTYALHRO MYPTYALHRO MYPTYALHRO MYPTYALHRO MYPTYALHRO MYPTYALHRO VYPYFYLHRO VYPYFYLHRO	( ( ( ( ( ( ( ( ( ( ( ( ( ( ( ( ( ( ( (	321 321 332 328 363 376 394 355 403	)

1 EEVE-ENEDE ENMIRKwppq-deleggeredhre laz 2 PSON-PDEHR EDVtrdtrghelsgeredhre Mer 3 EEVE-SNEDE EDUtrfp-n-rH-gereweahne ico	HI AKAEL DI AKIRG	( 3			
TOTAL STATE OF THE TOTAL STATE O	DIAKIRG				
TOTAL STATE OF THE TOTAL STATE O		(3	60	)	
	LIT AUT EM	( 3	71	)	
4 EREN-ACEMH VDEsrqk-v-sHETTEGHGSHLC LGO	HLARREI	(3	67	)	
	OFALHEA	(4	10	)	
5 KTIWODDVER WREerfenps aipqh-akwkyeGNGOKAGSIGO C WEST BOTTON B	GIARMET	(4			
6 EKAT-PNEKV FDEGhfides -gnikksdyrampesakkansyks	GLARME L	(4			
7 EKAF-PNEKV EDEGhfldes -gnfkksdyF MPESAERRMe VGE	A FATMOT	(4			
9 POHW-PEERE ERECTSKEN kgsidpy-vY LPEGNOPRNC IGM	REALMNM	` -		•	
9 POHW-PETER ERREITSKEN kgsidpy-vy LPEGNOPEN IGM	REALMIN				
10 PKYW-TEJEK ELLerfskin kdnippy-iy TPEGSEPRNO IGM	DESTANN	( 4	51	١	
ponw-proper greerisken kgslopy-vi legengrade in the control of the	DEST MINM	, ,		,	
12 PKYW-TEDEE ERBerfskk- kdsidpy-iv TPEGTEPKK IGM	DESTINAT				
13 PRYW-TENEK CCEerfskkn kdsidly-ry IPWGAGPRNG ISW	RESTANT				
14 POHW-TEPDE FREERFISKIN kdninpy-iY HPFGAGPRNG LGM		{ 4	162	,	
15 PRYW TEPEK TLEErfskkn kdnidpy-iv TPEGSOPKNO IS	REALVING	( 4	132	. 1	
16 QSLW-PEDEE BREEFFSIKE kdsinpy-ty LPEGTEPKNE 188	KENTMAM				
18 bkin-beffer firsten dazibb-mi refesseren in	Kt Driver				
CSB 10 CSB 11 CSB 12A CS	SB 12B				
			,	403	,
1 TTVFSTLYOKPDLKVav plgKTNYTPL NRCVGIVDLP Vi			•	403	-
2 EVARRALFGR Ep-ALSLGid ad-DVVWRRS LillRGIDHLP Vrl	.ag			412	
3 KIFFEELLPR E-kSVELSg PPRLVAT NEVGGPRNVP Erf	тка			414	
4 IVIDKEWLTR TOOFSLAP g-AOTOHKSEGIVSGVOALP LVV	opattka v		•		•
5 TLYECMALKHEEDFEDHtn-YELDIKEETLILKPEGFV.Vka	kskkipi g	gib	,	433	?
6 FLETTSHION E KLOSLve pkdLDITAVVANG fVSVPPSY 010	ripi n	nnn	•	4/3	'
7 FLEUTSILON EKLOSLve pkdLDITAVV NGfVSVPPSY Qlo	ripi		•	487	-
8 KAIFSVILRE I EFEMAQD p-eSYRNDHS RMVVOLAOPA-CVI	grrrtgv		(	450	)
9 KLANTKVLON ESFQPCke tq-IPLKLSR QGlLQPTKPI Il)	vvpr				
10 KLATIRVLON SSFKPCke tq-IPLKLSL GGllQPEKPV Vl)	vesr				
11 KLANIRVIONSFKPCke tq-IPLKLSLEGGlLOPEKPV-V11	vesrdgt v	sga	(	502	)
12 KLALIRVLON E-SFKPCke tq-IPLKLDT QGILQPEKPI VI)	vdsrdgt L	sge			
13 KLAVIRALONEE SFKPCke tq-IPLKLDN LPlLQPEKPI VI)	whlrdgi t	sgp			
14 KTALVELMONER - SFKLCke tg-VPLKLGK OG1LOPEKPI VI	cvvsrdgi i	rga			
15 KLALVRVION E SFKPCke tq-IPLKLRF GG1LLTEKPI VII	caesrdet v	sga	(	503	)
16 KLALVRVLÖNEE—SFKPCke tq-IPLKLNA QGLIQPEKPI VI)	(veprags v	nga			
17 KLALVRVIONSE—-SFKPCke tq-IPLKLTT QG1TQPEKPV VI	cilprdgt v	sga			
18 KVALVRVLON E TVQPCke te-IPLKLSK QGlLQPENPL L1	cvvsrdet v	sde			
CSB 12B					

FIGURE 1

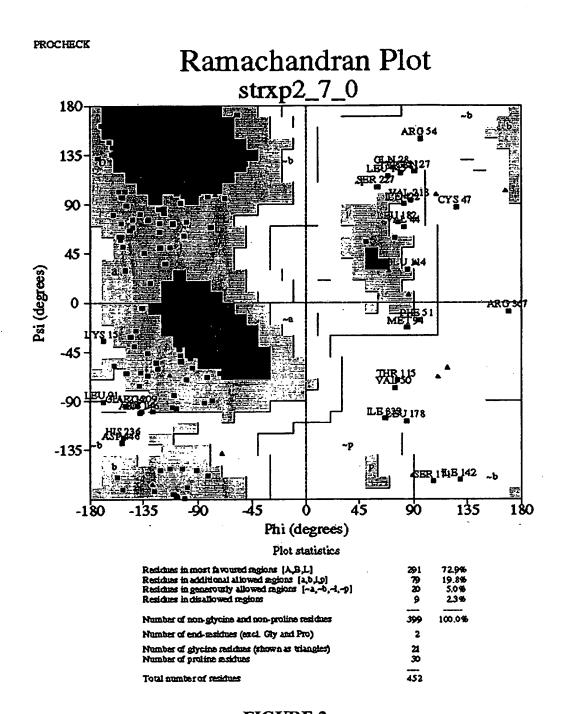


FIGURE 2

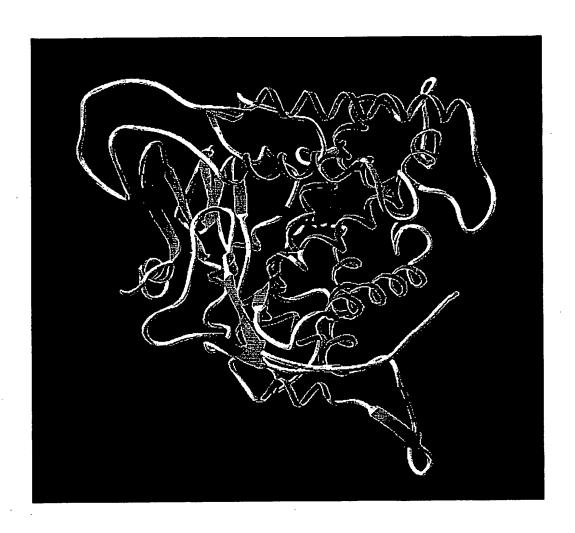
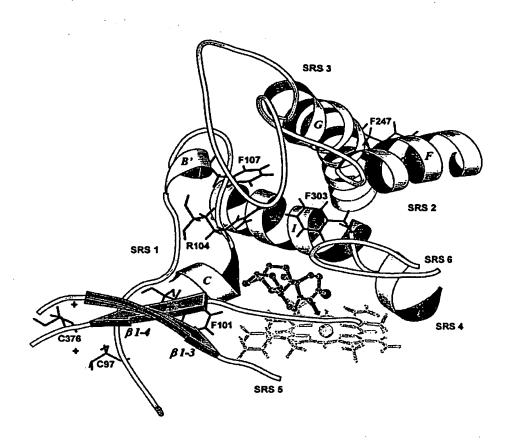
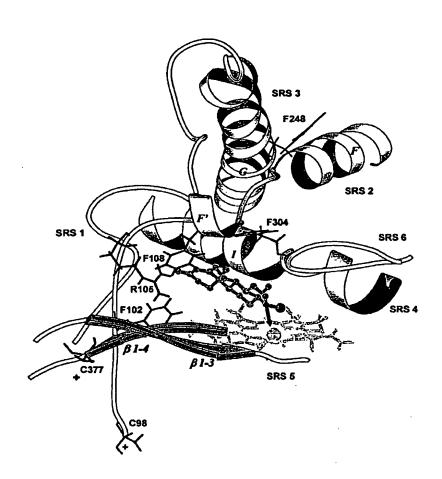


FIGURE 3



**FIGURE 4A** 



Testosterone

OH

16 
$$\alpha$$

HO

3A7

FIGURE 4B

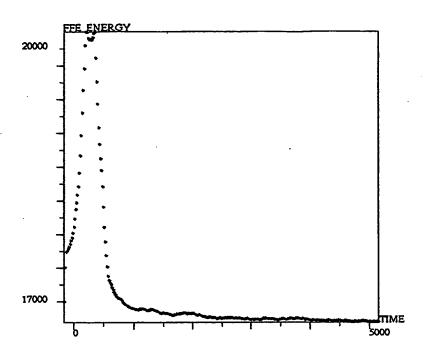


FIGURE 5